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PREDICTING SWITCH-LIKE BEHAVIOR IN PROTEINS USING LOGISTIC REGRESSION ON SEQUENCE-BASED DESCRIPTORS

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PREDICTING SWITCH-LIKE BEHAVIOR IN PROTEINS USING LOGISTIC REGRESSION ON SEQUENCE-BASED DESCRIPTORS

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PREDICTING SWITCH-LIKE BEHAVIOR IN PROTEINS USING LOGISTIC REGRESSION ON SEQUENCE-BASED DESCRIPTORS

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ABSTRACT

Predicting Switch-Like Behavior in Proteins Using Logistic Regression on Sequence-Based Descriptors

by Benjamin Strauss

Ligands can bind at specific protein locations, inducing conformational changes such as those involving secondary structure. Identifying these possible switches from sequence, including homology, is an important ongoing area of research. We attempt to predict possible secondary structure switches from sequence in proteins using machine learning, specifically a logistic regression approach with 48 N-acetyltransferases as our learning set and 5 sirtuins as our test set. Validated residue binary assignments of 0 (no change in secondary structure) and 1 (change in secondary structure) were determined (DSSP) from 3D X-ray structures for sets of virtually identical chains crystallized under different conditions. Our sequence descriptors include amino acid type, six and twenty-term sequence entropy, Lobanov-Galzitskaya's residue disorder propensity, Vkabat (variablility with respect to predictions from sequence of helix, sheet and other), and all possible combinations. We find the optimal AUC values approaching 70% for the two models of just residue disorder propensity and separately Vkabat. We hope to follow up with a larger learning set and using residue charge as an additional descriptor.

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TABLE OF CONTENTS

CHAPTER

LIST OF TABLES

LIST OF FIGURES

CHAPTER 1

Introduction

Amino acids are molecules that are often called the building blocks of life. In a biological system, these molecules are covalently connected together to form proteins, larger molecules that perform a function in an organism. Since many biological processes are initiated by a protein interacting with another molecule, understanding proteins is critical to understanding biology. Other molecules (ligands) binding to a protein can change the protein's function in a variety of ways, and these changes in function are an area of ongoing research.

1.1 Amino Acids

The function of a protein is determined by the amino acids that comprise it. Amino acids themselves are smaller molecules, made of a standard part and what is known an R-group or side chain, which differs between amino acids. These side chains give the protein their 3D structures. The basic structure of an amino acid is shown below, where R represents the side chain.

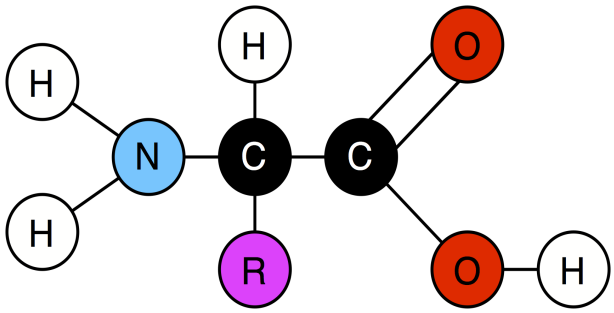
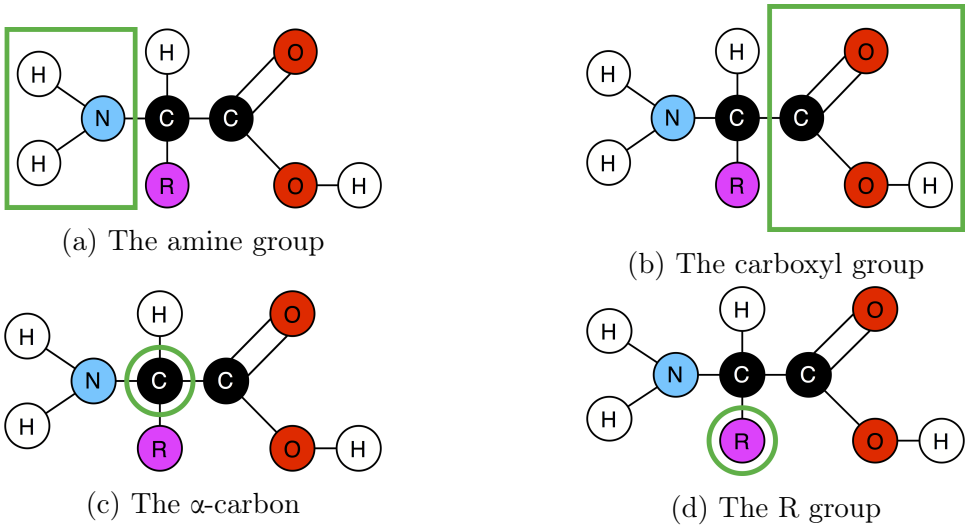


Figure 1: Two-dimensional structure of an amino acid.

There are four main parts to amino acids: the amine group, the α-carbon, the

carboxyl group, and the R group, and I have marked these in Figure 2:



(a) The amine group

(b) The carboxyl group

(c) The α-carbon

(d) The R group

Figure 2: The parts of an amino acid.

When amino acids bond together to form proteins, they are joined by peptide bonds to form what is called a polypeptide, which is a number of amino acids bound together in a chain.

1.2 Protein Structure

Proteins have four levels of structure, see Table 1. For identifying possible switches and allosteric regions, we mainly look at the primary and secondary layers.

Table 1: Levels of protein structure [1, 2].

Primary	Amino Acid Sequence
Secondary	Local Structure (Helix, Sheet, et cetera)
Tertiary	Overall Chain Structure
Quaternary	Interaction betweeen Multiple Chains

1.2.1 Molecular Sequence

When organized into proteins, amino acids are usually known as residues. This is when the amino acids bond to form the peptide chain, and they lose a water molecule. However, since this always happens in the forming of polypeptide chains, this detail is mostly irrelevant for computationally analyzing proteins. Note that the terms "protein chain", "residue chain", and "peptide/polypeptide chain" get used interchangeably in biology.

The first layer of protein structure is the amino acid residue chain sequence. We typically represent this computationally as a string of capital letters, where each amino acid is represented as a capital letter. Capital letters work well because there are 20 standard amino acids. There are also two "non-standard" amino acids which are represented by 'O' and 'U', respectively. Some letters also can stand for multiple amino acids, such as 'X' that can stand for any. 'B', 'J', and 'Z' as well as some Greek letters can stand for one of multiple amino acid types [6].

The two ends of the amino acid residue chain are referred to as amino terminus (N-terminus) and carboxyl terminus (C-terminus) respectively, and these are determined by the "free group" at that specific end. Amino acids each have two molecular connectors: an amine $-NH_2$ group and a carboxyl $-COOH$ group, and bonds between amino acids always occur between these connectors. If an amino acid has one of these groups not connected to another amino acid, it is called a free group. By convention, strings representing amino acid chains always start with whatever amino acid has a free amine group, which is also known as position 1 on the chain. The next amino acid is position 2, and the one after that position 3, et cetera until the carboxyl end of the chain.

The sequence of a protein is unique to that protein, and defines its structure and function, however many proteins have multiple chains of identical sequences.

1.2.2 Secondary Structure

The secondary structure of a protein is essentially defined by hydrogen bonding between amino acid backbones. Hydrogen bonding occurs between the carbonyl oxygen in Figure 1 and any hydrogen in the polypeptide. This is partly due to the fact that oxygen is highly electronegative, and partly due to the resonance structure shown in Figure 3:

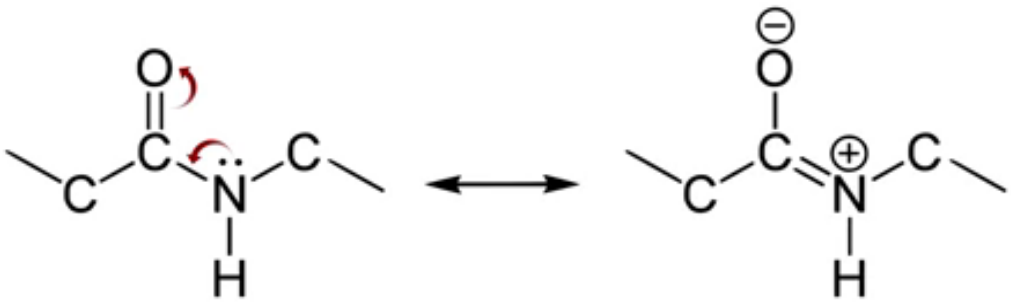


Figure 3: Resonance structure of amide linkage [4].

A resonance structure is where electrons can be described as both structures. This also stabilizes the backbone of the protein molecule.

There are two basic major types of secondary structure: helices and sheets. However, some proteins also have other structures. Both of these structures are fairly straightforward to visualize at the large scale. For example, α-helix appears as a helical coil, with each amino acid residue interacting with the residues 3.6 positions above or below it [2]. On the other hand, β-sheet appears as two polypeptide backbones being held parallel or anti-parallel to each other [4].

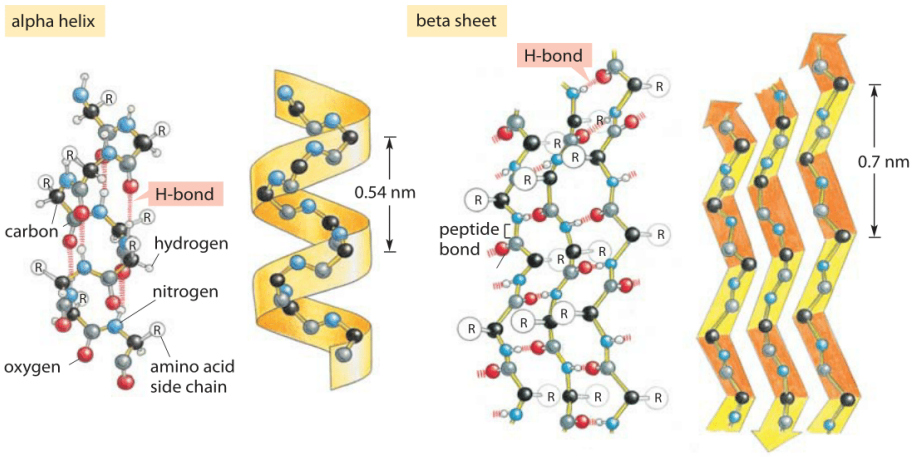


Figure 4: Schematics of α-helicies and β-sheets(anti-parallel) [5].

However, experimentally obtaining the secondary structure in detail is non-trivial. Luckily there are many programs designed to characterize protein topology from X-ray and NMR data, including secondary structure.

1.2.3 Tertiary Structure

Tertiary structure is determined by the R-groups, the part of the amino acids that makes the molecule unique. R-groups are comprised of hydrogen, carbon, nitrogen, oxygen, and sometimes sulfur or selenium, and are sorted into two main groups: polar and non-polar. This makes a difference in the 3-dimensional structure of a protein chain since water is a polar molecule, and the cytoplasm of cells (where proteins typically reside) is mostly water. Polar molecules interact with a polar solvent (like water in cells) and non-polar molecules do not. As a result, the polar R-groups tend to be on the outside of the protein and the non-polar R-groups cluster together on the inside, away from the water.

Polar amino acids are then further divided into three categories: acidic, basic, or neutral. Among the first two, ionic interactions are possible, while the latter can

participate in hydrogen bonding, including with water. These interactions can contribute to the protein's tertiary structure. Finally, if there are two cysteine residues that are physically near each other, the sulfur atoms in the R-groups can form a covalent bond, which also contributes to the tertiary structure, and possibly between chains with respect to quaternary structure [4].

1.2.4 Quaternary Structure

The final type of structure that proteins have, quaternary structure, is the result of interaction between multiple chains of amino acid residues. Note that typically the chains are not covalently bound to each other, so a protein with a quaternary structure is actually multiple molecules. (Proteins with only one chain are said to have no quaternary structure.) The chains involved may or may not all have the same primary sequence, but having the same primary, secondary, and tertiary structure is not uncommon of the chains in a protein.

An example of quaternary structure is a protein named 4JJX (RCSB-PDB [7] model) shown in Figure 5.

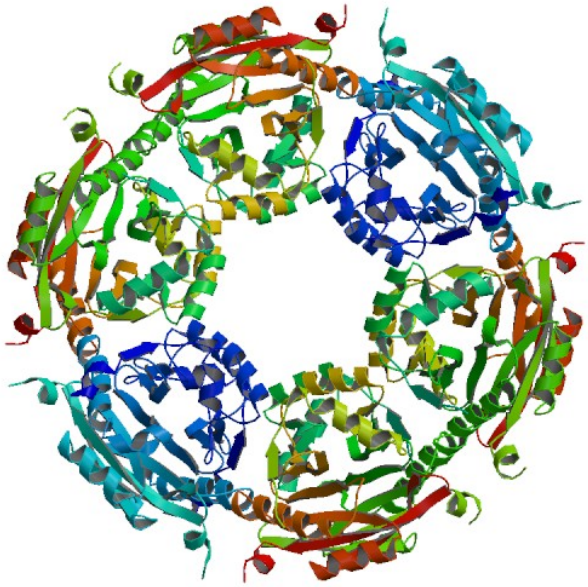


Figure 5: Protein 4JJX: Spermidine N1-Acetyltransferase from Vibirio Cholerae.

4JJX has 12 chains with identical sequence of amino acid residues. 4JJX also has a double-layered structure with each layer being comprised of a hexamer, or structure consisting of six residue chains. These chains are labeled 4JJX:A to 4JJX:L respectively, even though they all have (effectively) the same residue sequence.

1.3 Allosterism and Protein Switches

Protein conformational switches are regions of a polypeptide chain that undergo a significant structural change upon receiving a signal. As a result of this structural change, the protein then interacts with its environment differently (for example, new areas of the protein could be exposed to solvent). The potential signals consist of molecules binding to the chain covalently, or otherwise (such as hydrogen bonding, absorbing a photon, binding a drug, or engaging an entire cell via a surface receptor). And while many proteins bind other molecules and/or

become covalently modified; in order for a protein to be a switch, the structural change must be stimulus induced [8].

The classic example of this is the protein hemoglobin (typically found in blood). In the protein-ligand reaction, the oxygen molecule O_2 binds to the hemoglobin, and as a result, makes it easier for other oxygen molecules to further bind. Other molecules that bind to proteins in this manner can affect protein structural features, such as side-chain packing, secondary structure mobility, domain movement, and oligomerization, depending on where and how they bind to the protein [9].

1.4 Stating the Problem

Protein allosterism presents a giant puzzle for researchers as the extent of allosteric behavior in proteins is not well understood. Furthermore, we do not know if protein allosterism is a boolean on/off switch based on the presence of one specific ligand, or a switch statement based on one of many potential ligands. And of course it may be that in some situations multiple ligands can bind to one allosteric region on the same protein.

In this sea of unknowns, we have decided it is best to start unraveling how this mechanism works by trying to identify possible protein switches. We detail this in the next sections.

CHAPTER 2

Objective

Determining switch-like behavior requires us to define it. We decided upon the following definitions. Note that residues Unassigned are classified by an absence of secondary structure type by the gold standard database DSSP [10].

Definition 1. *An amino acid residue exhibits switch-like behavior iff it, under different conditions, has two or more of the following categories of secondary structure: Helix, Sheet, and Other, or is Unassigned.*

From here, we split switch-like behavior into two types:

Definition 2. *An amino acid residue is an assigned switch iff under different conditions, has two or more of the following categories of secondary structure: Helix, Sheet, Other.*

Definition 3. *An amino acid residue is an unassigned switch iff it has one of only two classes of secondary structure, with one category being Unassigned.*

CHAPTER 3

Methods

3.1 Identifying Sequence-Based Descriptors

To look for allosteric regions, we chose a pattern-based approach of analyzing already-known allosteric regions for patterns based on five specific criteria:

Table 2: The sequence-based descriptors for the search for allosteric regions.

Residue Sequence	Sequence of types of side chains on the amino acids that make up the proteins.
6-Term Sequence Entropy (E6)	First order approximation of local flexibility of the molecule, high values suggest high mobility of that residue.
20-Term Sequence Entropy (E20)	Alternative first order approximation of local flexibility of the molecule, high values suggest high mobility of that residue.
Lobanov-Galzitskaya (IsUnstruct)	Probability than a residue will be disordered.
Vkabat	Variability of predicted secondary structure.

3.1.1 Residue Sequence

The residue sequence is our first descriptor, and our only qualitative one [11]. The Uniprot FASTAs we used classify amino acids with respect to the standard 20, so the residue sequence gets modeled as an array of 20-valued enums.

3.1.2 Sequence Entropy

Sequence Entropy (also known as "Shannon Information Entropy") is a type of information entropy, which is related to thermodynamic entropy [12]. Additionally, in this 2005 paper by the Lustig group, low sequence entropy was correlated to

inverse packing density (a physical measure of local flexibility). As it turns out, sequence entropy at a particular residue k, (denoted as S_k) is not difficult to calculate, as given by the equation

$$S_k = -\sum_{j=1}^{20} P(j,k)\ log_2(\ P(j,k)\ ) \tag{1}$$

where $P(j,k)$ is the probability of how often residue k is present in a set of aligned residues. The 20 values for j come from the 20 standard [12] amino acids (we do not count Pyrrolysine or Selenocysteine). Note that an alternative version of this calculation can be done where j goes from 1 to 6; in this case, each value for j represents a group of amino acids. The amino acids are categorized [3] in Table 3:

Table 3: Groupings of amino acids relevant to E6 sequence entropy[3].

Aliphatic	Alanine, Cysteine, Isoleucine, Leucine, Methionine, Valine
Aromatic	Phenylalanine, Histidine, Tryptophan, Tyrosine
Polar	Asparagine, Glutamine, Serine, Threonine
Positive	Lysine, Arginine
Negative	Aspartic Acid, Glutamic Acid
Special	Glycine, Proline

3.1.3 IsUnstruct (Lobanov-Galzitskaya)

The Lobanov-Galzitskaya method, IsUnstruct, is a way of predicting with amino acid residues that are disordered solely from the residue sequence [13]. The output of the IsUnstruct method is a number from 0 to 1 for each residue, which is then interpreted as the probability that that residue will be disordered.

For our purposes, we use IsUnstruct as a black box function that takes in a protein chain sequence and outputs a value. This Ising model application comes

from statistical physics (as Ising models were originally used to predict statistical mechanical phenomena) and the final value is derived as the following ratio:

$$p_{i,1} = \frac{Z_{i,l}}{Z} = \frac{\sum_{j=i}^{M} \; s_{ij} \; \cdot \; e^{\frac{-E_j}{kt}}}{\sum_{j=i}^{M} \; \cdot \; e^{\frac{-E_j}{kt}}} \tag{2}$$

where E_j is defined as

$$E_j = \sum_{i=1}^{L} \; w(a_i, s_{ij}) \; + \; e_b \cdot b \; + \; t_n \cdot e_n \; + \; t_c \cdot e_c \tag{3}$$

Equations 2 and 3 have been relabeled from Lobanov and co-workers [14].

Table 4: Variables of the Lobanov-Galzitskaya equations.

a_i	type of amino acid residue
b	number of bordering residues
e_b	energy of the residue's borders
e_c	energy of initiation of the c-terminus
E_j	energy of the microstate
e_n	energy of initiation of the n-terminus
k	Boltzmann constant
L	length of the protein chain
s_{ij}	the state of the ith residue at the jth conformation
T	temperature
t_c	0 if c-terminus residue is ordered, else 1
t_n	0 if n-terminus residue is ordered, else 1
$w()$	given in a table in [14]

3.1.4 Vkabat

Vkabat is our way of calculating how diverse the range of secondary structures are [15] and is defined [3] by the following function:

$$Vkabat = \frac{k \times N}{n_1} \tag{4}$$

In this equation, k is the number of secondary structure classes predicted for that residue. Here we can classify up to three categories, helix, sheet and other. N is the total number of possible chains, or how many predictions we are making. The variable n_1 is the number of times that the most common type of secondary structure occurs in all of the predictions made. For our purposes, $N = 15$, since we use the 15 algorithms for calculating the prediction of secondary structure originally applied by Saravanan and Selvaraj [16]. The minimum and maximum values for Vkabat are 1 and 9, respectively.

3.2 Applying Logistic Regression

Logistic Regression is a mathematical way of determining the probability of a binary event occurring based on one or more parameters. Applying the aforementioned descriptors, our binary event describes whether or not a protein chain residue in question has switch-like characteristics. Using logistic regression with proteins is not new, and was done previously by the Lustig group predicting from sequence which R groups were on the inside of a folded protein [17] as well as residues of one protein interacting with residues on another.

To implement logistic regression, we first assemble learning and test sets of protein chains. From this we plan to calculate switch-like regions, depending on the descriptor value(s). Our quantitative descriptors are sequence entropy, IsUnstruct, and Vkabat. It is important to note that the odds is not the probability, although it can be derived from the probability p as such:

$$\text{Odds} = \frac{p}{1-p} = e^{\sum_{i=1}^{n} k_i x_i} \tag{5}$$

Here x_i is the quantitative descriptor and k_i is the associated weighting coefficient [18, 19]. However, the odds in this raw form do not give a linear correlation with the descriptor data. So to make matters simpler, most often the odds are transformed into the "log odds" (literally the natural log of the odds) which turns the formula into a linear polynomial:

$$\text{Log Odds} = \ln \text{Odds} = \ln\left(\frac{p}{1-p}\right) = \sum_{i=1}^{n} k_i x_i \tag{6}$$

The log odds for each residue are given by the following coefficients and descriptors [17]:

$$\eta = \beta_0 + (\beta_1 \times \text{E6}) + (\beta_2 \times \text{E20}) + (\beta_3 \times \text{IsU}) + (\beta_5 \times \text{VK}) + \sum_{i=1}^{19} (\beta_{i+4} \times X_i) \tag{7}$$

Here the β terms are constants (and η is the symbol for the log odds). The last terms a of equation 7 are qualitative descriptors. Each of the different types of amino acid have their own unique identifier. Depending on what type of amino acid is present, one X_i will be 1, and all the rest will be 0. (Note that β_0 should be representative of valine.) One can rearrange the terms in equation 5 and noting equation 7 get the following:

$$p = \left(\frac{e^{\beta_0 + \beta_1 E6 + \ldots}}{1 + e^{\beta_0 + \beta_1 E6 + \ldots}}\right) \tag{8}$$

The other acronyms for descriptors are as follows:

- E6 is a six-term sequence entropy
- E20 is a 20-term sequence entropy
- IsU is IsUnstruct
- VK is Vkabat

CHAPTER 4

Data

4.1 Choosing Learning and Test Sets

We chose N-Acetyltransferases and Sirtuins respectively because there is some documentation of possible switch behavior among them [20]. In addition it should be noted that N-Acetyltransferaces and Sirtuins share similar regulatory and functional features.

Originally, the chains were clustered with Pisces, at 98% or greater sequence identity [8]. We got our initial chains to do this clustering from Khun (personal communication) which lead to 34 usable clusters (some of which later were determined to be part of larger clusters). We added to these clusters using the results of RCSB-PDB keywords searches: "Spermidine" and "N-Acetyltransferase."

To further refine the clusters, we discovered that JPred, used in the VKabat algorithm, lists all the protein chains that have a similar sequence to the sequence entered. (From here, it offers the opportunity to use a known chain's secondary structure sequence instead of running the prediction). It became immediately obvious that this could be used to find similar chains, since they were listed in ascending order by blast E-value. (The lower the blast E-value, the more similar a chain was to the input sequence and vice versa.)

Thus, we entered each dominant chain's sequence into JPred and then went down the list of chains, checking each chain's RCSB-PDB FASTA sequence manually until a chain did not resemble the dominant chain. It was quickly discovered that once one sequence that did not resemble the dominant chain, none

of the ones after would. This latter method identified an additional cluster (4KVO and related sequences) resulting in a total of 48 working clusters. See appendix A.16. Note 44% of clusters are 5 or less, while 84% are ten or less. These are comparable to cluster sizes associated with determining C_{alpha} displacements for 3D X-ray structures crystallized under different conditions [21].

The test set clusters of Sirtuins were previously assembled [20]. However it was later determined to use "4IAO" instead of "4AIO". The same JPred-based method was applied to the Sirtuins and no changes resulted when compared to the original clusters. We wound up with five usable clusters of Sirtuins, as shown by Table 5.

Table 5: Test set clusters, dominant chain is the original chain of interest.

Dominant Chain	**Other Chains**
2B4YA	2B4YB, 2B4YC, 2B4YD, 2NYRA, 2NYRB, 3RIGA, 3RIGB, 3RIYA, 3RIYB, 4F56A, 4F56B, 4F4UA, 4F4UB, 4G1CA, 4G1CB, 5BWLA, 4HDAA, 4HDAB, 6EQSA, 6EQSB, 6EQSC, 6EQSD, 5XHSA
2HJHA	2HJHB, 4IAOA
4IG9A	4IG9C, 4IG9E, 4IG9G, 4KXQA, 4IF6A, 4I5IA, 4I5IB
4L3OA	4L3OB, 4L3OC, 4L3OD, 4RMHA
5BTRA	5BTRB, 5BTRC, 4ZZHA, 4ZZIA, 4ZZJA

The next challenge was identifying switches. Since we define switch-like behavior as a residue changing its secondary structure: we had to determine which residues exhibited this behavior in the learning set and in the test set.

To do this, we decided to compare each dominant chain (the chain that we were trying to determine switch-like regions for) to chains with identical or nearly-identical sequences, resulting in clusters. It is important to note that in order for us to use a protein chain in the regression, we needed to have at least one chain

that was similar to compare it.

4.2 Modeling Proteins With Java

Starting out, we had python scripts to calculate the entropy and Vkabat of a given residue sequence, and we had the Lobinov-Galzitskaya IsUnstruct program written in C. However, we had no way of organizing this data. My goal was to automate the entire process, and create a program that if given a list of RCSB-PDB IDs, could generate a data set to be used in the Logistic Regression without any manual assistance. While we did not achieve complete automation, see 6.1.1, we came very close and automated most of the data set generation.

Java was used to write this intigrative program. Java's object-oriented approach meant one could model the pieces individually, with each object holding the data about itself. Once we had the model, it would then be simpler, if not trivial, to gather the requested data from it and display it in whatever form we found most useful and intuitive.

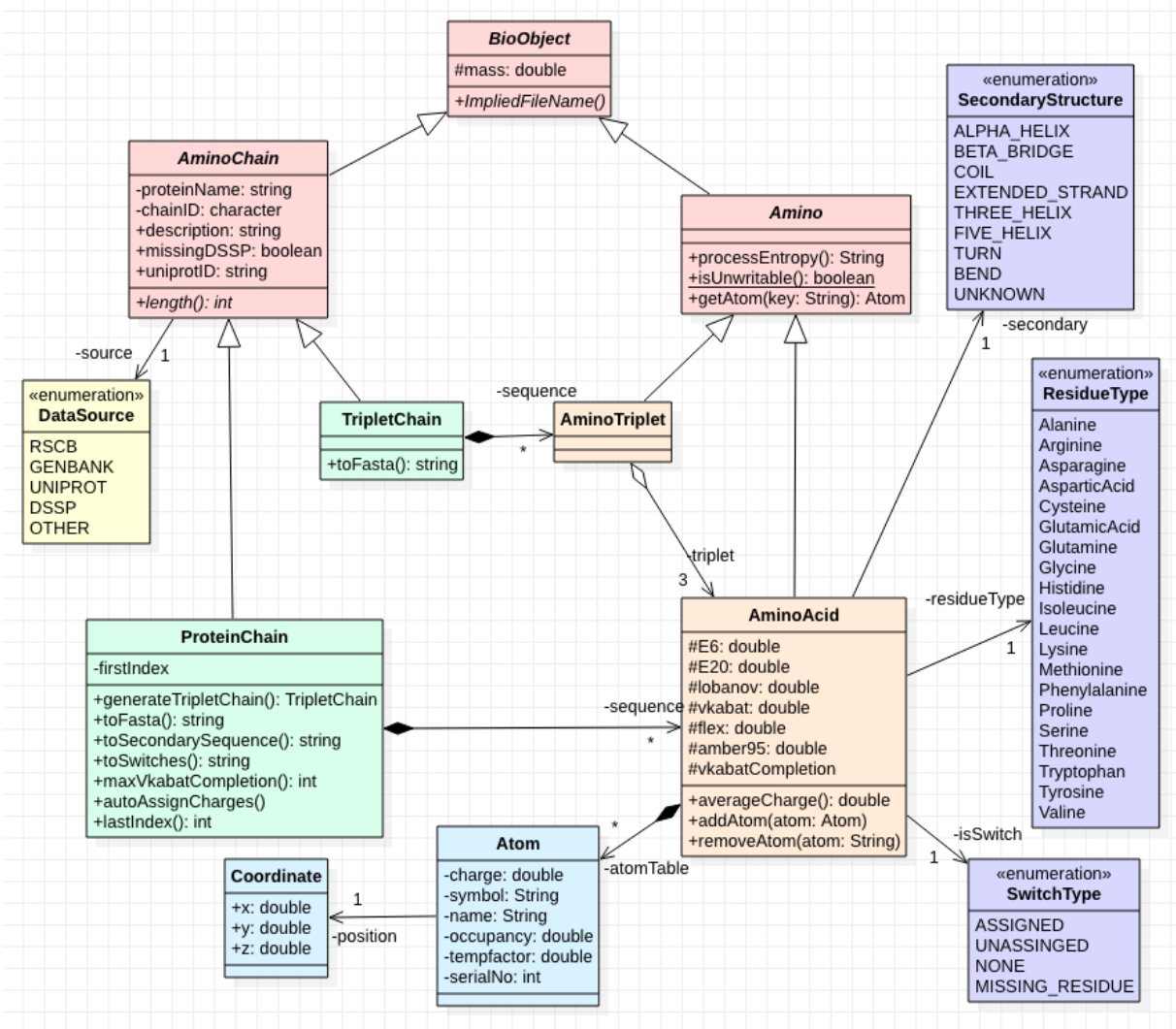


Figure 6: Class diagram of the protein chains.

When it came to clustering, we went with the model in Figure 7.

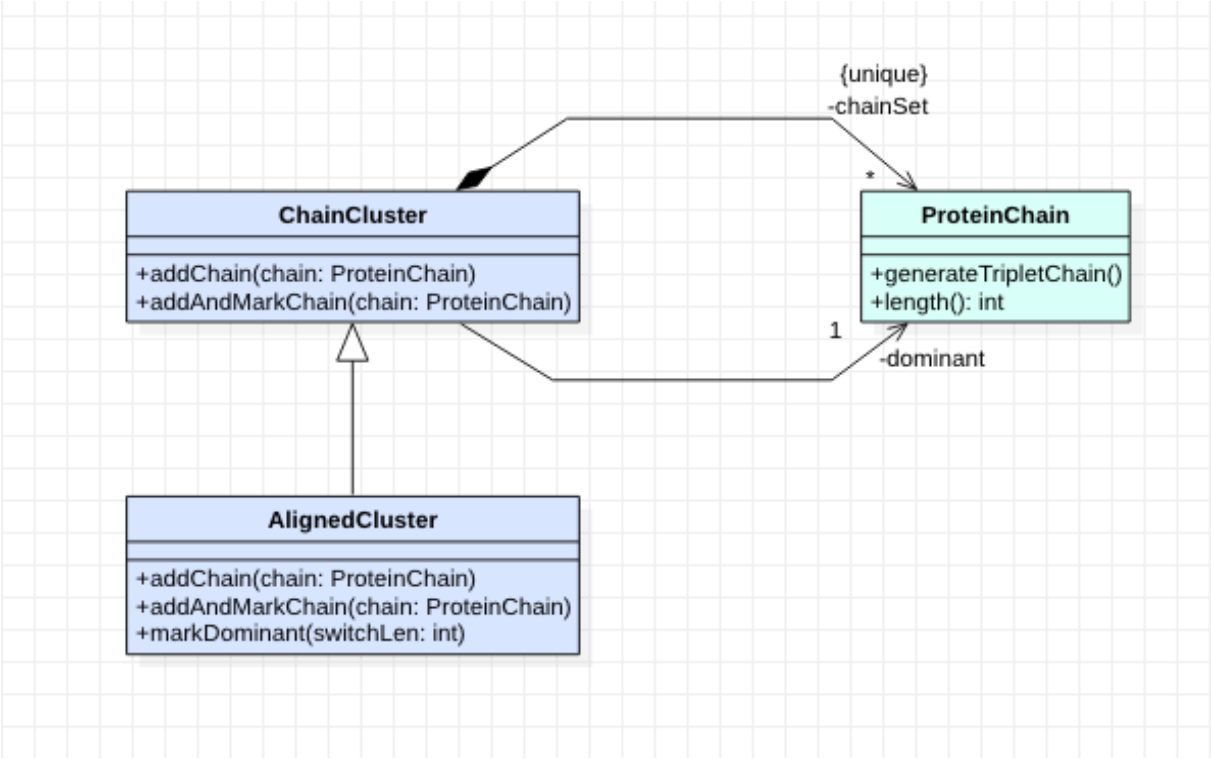


Figure 7: Class diagram of the clusters.

4.3 Data Set Generation

Generating the data sets used in the logistic regression involved downloading data, saving the data, and then writing it out in a CSV format, which the Logistic Regression python script could then use.

4.3.1 Downloading FASTAs

We initially planned to use the FASTAs from the RCSB-PDB, and did use these for the early runs of our project. However there may be a problem: sometimes parts of the residue chains were missing, and the RCSB files in no way indicated where and how big were the gaps. Given how algorithms like IsUnstruct and Vkabat base their results on sequence alone, this meant that the RCSB-PDB FASTAs were

problematic for our purposes.

From here, we turned to GenBank and Uniprot, and we modified the program to allow the user to specify the FASTA source (and we set it to Uniprot by default). Uniprot FASTAs turned out to be more robust than their GenBank counterparts, as some of the Vkabat component algorithms ran into trouble when using the GenBank FASTAs. Sometimes because they could not handle a residue 'X' (Uniprot FASTAs did not have 'X' in them, but used the closest standard amino acid), and sometimes apparently for other reasons.

Using Uniprot however created another problem: the Uniprot did not use the RCSB-PDB identifiers. This meant that in order to get the Uniprot sequence from an RCSB-PDB identifier, one had to go to the RCSB-PDB page and parse the data to find where the Uniprot identifier was listed. For the most part this was easy since when parsing the RCSB-PDB HTML, the Uniprot identifier was always clearly marked. But with this approach, we still ran into trouble.

While this approach always obtained a Uniprot ID, the Uniprot ID was occasionally incorrect. This happened when a RCSB-PDB page had multiple Uniprot IDs for the same RSCB-PDB identifier, and from the RSCB-PDB identifier alone, there was no way to tell which Uniprot ID we wanted. To get around this issue, we modified the way that the cluster file is read: allowing the user to put a Uniprot ID after the RCSB-ID to ensure that that Uniprot ID will be used. (If no Uniprot ID is entered, the program will look up the Uniprot ID in the aforementioned way if necessary.) When doing this, the program will always obtain the first Uniprot ID on the page.

After downloading the FASTA sequence, the sequence will be saved in "files"

under a directory named after where that FASTA came from, so it does not have to be downloaded again.

4.3.2 Obtaining Secondary Structure Data

To obtain the secondary structures of a protein chain, we used the DSSP files, which are held locally under "files/DSSP/". When assigning secondary structures to a protein chain, we ran into the problem that sometimes a DSSP file could not be found. (The reason, as it turned out, is that we did not have all of the DSSP files, and downloading the rest fixed this).

If secondary structures cannot be assigned from the DSSP files, the program is also equipped to assign them from the headers in the appropriate PDB files from RCSB (in which case the user will be alerted). This RCSB secondary structure information is stored in "files/ss.txt". Unless one is working with a FASTA sequence from PDB or GenBank, using PDB annotated secondary structures is sub-optimal, since a PDB sequence must be used as an intermediary (the sequence from the PDB corresponds with the PDB FASTA and may not match other FASTAs) and aligning RCSB sequences to other sequences can be error-prone, (see Table 7 for why this is a problem and 4.3.3.1 for how we deal with it).

Either way, secondary structures are interpreted as follows. The code that does this can be found in bio.SecondaryStructure

Table 6: Characters found in the .dssp files denoting secondary structure.

DSSP-Char	**Secondary Structure**	**Structure Category**
B	Beta Bridge	Sheet
E	Extended Strand	Sheet
G	Three Helix	Helix
H	Alpha Helix	Helix
I	Five Helix	Helix
S	Bend	Other
T	Turn	Other
(blank)	Other or Random Coil	Unassigned

4.3.3 Aligning Sequences

A huge problem when dealing with proteins is that different databases have slightly different sequences for the same protein chain, even when ignoring the sequence gaps in the RCSB-PDB. To do this project, we used four different sources for protein sequences: RCSB-PDB, GenBank, Uniprot, and DSSP. This meant that for a given chain, such as 4UA3:A (a chain that gave us a lot of trouble), there could be four different sequences, as in Table 7:

Table 7: 4 Different Sequences of 4UA3:A.

Source	**Sequence (4UA3:A)**
RCSB-PDB	XSRRMKTQEIKNVTLEDVDFLKNLGVWVEIYHHLEKGLLQQCFNLVKKNMEALYRQS SFGWDDSEKLKEMEMEKLEYICIFEKTSKKLVGFLSFEDTVEAGLTCLYIYEIQLDE HIRGRNVGKWLLKNASILAYRRNLKYIFLTVFSANLNALNFYHHFDFVPHESSPQEK KFRSGKVIHPDYYILYTKSRKDW
GenBank	XSRRXKTQEIKNVTLEDVDFLKNLGVWVEIYHHLEKGLLQQCFNLVKKNXEALYRQS SFGWDDSEKLKEXEXEKLEYICIFEKTSKKLVGFLSFEDTVEAGLTCLYIYEIQLDE HIRGRNVGKWLLKNASILAYRRNLKYIFLTVFSANLNALNFYHHFDFVPHESSPQEK KFRSGKVIHPDYYILYTKSRKDW
Uniprot	MHFLKQYLFYSPRRMKTQEIKNVTLEDVDFLKNLGVWVEIYHHLEKGLLQQCFNLVK KNMEALYRQSSFGWDDSEKLKEMEMEKLEYICIFEKTSKKLVGFLSFEDTVEAGLTC LYIYEIQLDEHIRGRNVGKWLLKNASILAYRRNLKYIFLTVFSANLNALNFYHHFDF VPHESSPQEKKFRSGKVIHPDYYILYTKSRKDW
DSSP	SRRX VTLEDVDFLKNLGVWVEIYHHLEKGLLQQCFNLVK KNXEALYRQSSFGWDDSEKLKEXEXEKLEYICIFEKTSKKLVGFLSFEDTVEAGLTC LYIYEIQLDEHIRGRNVGKWLLKNASILAYRRNLKYIFLTVFSANLNALNFYHHFDF VPHESSPQEKKFRSGKVIHPDYYILYTKSRKDW

The fact that all these sequences could be different ('*' denotes something missing from the DSSP file) meant than when using the same sequence from any two sources, the sequences would have to be reconciled. Most of the possible problems that arose are visible from looking at the different sequences from 4UA3:A, and we break them down as follows:

The first kind of problems we faced were **Index Problems** RCSB-PDB and GenBank sequences have the same indices, and DSSP has index numbers that align with Uniprot. The trouble is that RCSB-PDB/GenBank and Uniprot/DSSP do not

match. These sequences not only tend to start/end at different residue positions, and as mentioned earlier, RCSB-PDB/GenBank can contain undeclared gaps in the FASTAs.

Unknown Residues also caused problems. GenBank and DSSP list non-standard residues as 'X' (selenomethionene is the most common reason for 'X') but RCSB-PDB and Uniprot use the closest standard residue. (4UA3:A is an exception to this rule, as the RCSB-PDB sequence contains an 'X' at the beginning, which corresponds not to an amino acid residue, but to an acetyl group.) Having an 'X' residue in a sequence would cause some of the Vkabat algorithms to crash.

Residue letter mismatches were also far from unheard of, even if neither was 'X'. We are unsure if this was a data-entry typo. DSSP uses **b** as a residue letter to denote a cysteine with a sulfur-sulfur bonded to another cysteine. This was an easy fix once we knew that it was happening.

4.3.3.1 A FASTA alignment algorithm

The solution to all of these problems was to create a Java class with static methods specifically for aligning residue sequences (bio.tools.SequenceAligner). Unlike normal string alignment algorithms, the purpose of this algorithm is to differentiate (as accurately as possible) between what is an unmarked gap in a sequence and what is a normal mis-match. Given that no table of sequence alignments exists (at least that we were able to find), one has to guess, and thus by the very nature of the algorithm, perfection is not guaranteed.

The first step in the sequence alignment algorithm is to figure out a base sequence that matches. The algorithm takes two strings of characters, each representing a residue sequence. From here, we look in the first sequence for a

unique sub-sequence of K residues. Then we look for the same string in the second sequence. If the second sequence also has a unique sub-sequence of K residues, we align the chains based on this sub-sequence, if not, we search for a new unique sub-sequence of K residues in the first sequence.

With the initial alignment, choosing a good K is critical. For a sequence of K residues, there is a 1 in 20^K chance that the sequence will happen randomly in the other protein, so a high K means a lower chance of error. However, if K is too high, errors in the sequences will mean that no match can be found and the alignment will fail. Thus the challenge is choosing the right value for K. We went with K = 32, (although a java programmer executing the alignment algorithm can specify a different value for K).

With K = 32, this means that the chance of giving a false alignment is 1 in 20^{32}, or roughly 1 in 4.3×10^{41}, which is fairly small. Even when looking at sub-sequences of a sequence of 1000+ residues, the chance that there will be a mis-match by chance is 1 in 4.3×10^{38}, which is still negligible.

The second part of the algorithm requires a bit more guesswork. bio.tools.SequenceAligner has a method called superAlign(), which is designed to differentiate between unmarked gaps in sequences and residues that are marked differently in different sources. There is no way to know for sure, but this algorithm makes estimates based on the length of mis-matched regions, using the assumptions that data mis-matches are fairly uncommon and that unmarked gaps are usually not small.

From this, if a large number of residues in one sequence do not match the residues at those same indexes in the other sequence, it is more likely that an

unmarked gap is the cause rather than a data conflict. If it's only one or two residues that do not match, then it is most likely a data conflict and can be ignored. In areas that only match in part, the algorithm has to determine if more residues match or mis-match, and then decide whether it is a gap, or data conflict, based on the number of mis-matching residues and the closest matching regions.

When dealing with what are determined to be gaps, the superAlign() method aligns segments first by inserting blank residues, starting with the largest (anything size 32 or larger) and moving down aligning smaller and smaller segments until it reaches segments of size 4. We chose the number 4 specifically because it is the smallest number of residues seen here in any FASTA to be separated from the true sequence by an unmarked gap. The final step is then to go through both sequences, and remove all blank residues that have a blank residue at the same index in the other sequence.

4.3.4 Lobanov-Galzitskaya's IsUnstruct

Of the descriptors we used, IsUnstruct was the second-easiest to obtain (after the sequence). Lobanov and Galzitskaya [13, 14] conveniently made IsUnstruct a C program, which meant we could run it locally, and since the source code was available, it was not too difficult to translate the entire program into Java. The code for the Java version of IsUnstruct is located in the package bio.tools.isUnstruct, and gives the same results as its C counterpart. This was tested on multiple occasions, including against propensities calculated with the C version for the protein chain 5BTR:A by Lustig, Wong, and Graham [20].

4.4 The Python Scripts

Obtaining the descriptors regarding entropy and Vkabat involved using Lustig Group Python scripts that had been written by my colleagues, Jonathan Oribello and Saira Montermoso. These scripts were not translated into Java, but run from Java as Python scripts. Java would then read in the results.

Getting these scripts to run was difficult because they required a newer version of Python than was installed. We do not know what the minimum Python requirement is, but Python 3.7.0 is known to work. When running the Python scripts, it is critical to specify the path for Python; if the wrong version of Python is used, the scripts will NOT work! The program uses the default Python path of "usr/local/bin/python3" (which works on Mac OS) but another path can be specified with the bio.util.PythonScript.setPythonPath() method.

Another requirement to run the Python scripts is to have all of the packages installed. The easiest way to do this is with pip, as this will tell you if the package is already installed. These packages include the following, although some may be installed by default.

- argparse
- Bio
- Bio.Blast
- collections
- csv
- htmlement

- lib
- logging
- numpy
- os
- pandas
- requests
- requests_toolbelt.multipart.encoder
- subprocess
- sys
- time

Finally, the scripts are designed to work with the Java program and not designed for standalone use. For these scripts to work properly, they must be run from the SwitchPrediction folder. All the paths to folders (and thus the data that they use) are based on this.

4.4.1 Entropy Scripts

To calculate the entropy values E6 and E20, the Java program executes a pair of Python scripts. The first of these is "getBlast.py" or "getBlastUniprot.py", which downloads the blast data. The script called depends on what the FASTA source (a variable internal to the program, e.g. RCSB-PDB FASTA) is set to: DSSP or Uniprot FASTAs will mean "getBlastUniprot.py" is called. Else, "getBlast.py" will

be called. This downloads the blast file and saves it in the proper folder within "scripts/blast/". After this, "calculate_entropy.py" is called, which calculates the E6 and E20 from the blast file. The Java program will then read this in, and assign E6 and E20 to the chain.

Since there are 22 proteinogenic amino acids, the Java code also contains an E22 value. However, the program has no way to calculate an E22 value, and the feature was unused in our project. To use the E22 value, one will have to calculate E22 with some other method, and then modify the logistic regression script to make use of E22.

4.4.2 Vkabat Script

Our Vkabat script is called "neo-vkabat.py" (to differentiate it from the original version made for a different project). When run, neo-vkabat obtains Vkabat data in the following order: GOR, DPM, GOR3, PHD, PREDATOR, HNN, MLRC, SOPM, JPred, then PROF, SSPRO, YASPIN, JNET, and PSIPRED via SymPred, and finally DSC. Neo-vkabat can be finicky, and often times one or more prediction algorithm will fail.

These algorithms can fail for various reasons, and it is not always clear why any given algorithm failed. When the prediction algorithms fail, they do not always fail consistently, that is, the same algorithm might fail for a given protein chain at one time and succeed at another. We do not know the reason for this, however we think it might be linked to the workload of the server in question. (There was no way for us to know the workload of the server).

Some algorithms are more robust than others, and some have a limit to the length of the chain that they can analyze. JPred has a limit of 800 residues, and

will not run on longer chains.

To solve this problem, we created the class bio.tools.VkabatRecoveryModule. VkabatRecoveryModule is used through the “patch” command of the JBioMain user interface, and will look in the “patches” directory, under the sub-folder that the fasta source is set to. To patch a Vkabat file, follow the steps below:

1. Run the secondary structure prediction algorithm online.
2. Copy the output into a text file with the name [protein+chain]-[algorithm].txt. (For example if 1S7F:A from a uniprot fasta fails JPred, then the patch would be “1S7FA-JPRED.txt”).
    - For JPred results, click “View simple results in HTML.”
    - For Sympred results use "SYMPRED+" for the algorithm.
3. Place that file in the "patches" directory under the sub-folder which corresponds to from where the sequence came.
4. From JBioMain, run “src” and enter the name of the sub-directory where your patch is. (Only the name, not the path).
5. From JBioMain, run “patch”.
6. From JBioMain, run “redo-vk” to re-assign the Vkabat values along with the patched data.

When run VkabatRecoveryModule, checks what secondary structure prediction data is in the Vkabat file by looking at the csv header, as so not to duplicate data already in the file if the patch command is run twice.

VkabatRecoveryModule does not read patches for all secondary structure prediction algorithms, just the ones that gave us trouble: PROF, SSPRO, YASPIN, JNET, PSIPRED, PHD (via Sympred), JPRED, MLRC, YASPIN, PROF, PHD, and PsiPred. Please make sure that the patch source is all uppercase on the patch file names.

The patches that we used are shown in Table 8:

Table 8: Vkabat patches needed in both the learning and test sets.

Chain	**Patches**
1N71A	SYMPRED+ (PROF)
1S7FA	JPRED
1XEBA	SYMPRED+ (PROF)
2B5GA	JPRED
2HJHA	SYMPRED+ (PROF, SSPRO, YASPIN, JNET, PSIPRED)
2REEA	JPRED, MLRC, SYMPRED+ (PROF, SSPRO, YASPIN, JNET, PSIPRED)
2WPWA	SYMPRED+ (PROF, SSPRO, YASPIN, JNET, PSIPRED)
3N37A	PHD, SYMPRED+ (PROF, SSPRO, YASPIN, JNET, PSIPRED)
3W6SA	JPRED
4AVAA	SYMPRED+ (PROF, SSPRO, YASPIN, JNET, PSIPRED)
4EABA	JPRED
4HNYA	JPRED, SYMPRED+ (PROF, SSPRO, YASPIN, JNET, PSIPRED)
4IG9A	SYMPRED+ (PROF, SSPRO, YASPIN, JNET, PSIPRED)
4KVOA	JPRED, SYMPRED+ (PROF, SSPRO, YASPIN, JNET, PSIPRED)
4KVXA	JPRED
4L3OA	PHD, SYMPRED+ (PROF, SSPRO, YASPIN, JNET, PSIPRED)
4PV6A	JPRED
4UA3A	JPRED
5BTRA	SYMPRED+ (PROF, SSPRO, YASPIN, JNET, PSIPRED)
5K04A	SYMPRED+ (PROF, SSPRO, YASPIN, JNET, PSIPRED)
5WIFA	JPRED
5YGEA	JPRED

Note that for JPred, when we had FASTAs over 800 residues long, we broke

sequences into 780-residue chunks because Uniprot FASTA lines are 60 residues long ($60 \times 13 = 780$).

CHAPTER 5

Results

5.1 Evaluating Descriptor Performance

We used ROC (Receiver Operating Characteristic) statistics to evaluate which descriptors worked the best. Our logistic regression algorithm generates a probability (see equation 8) for every residue that that specific residue is a switch. From this, we totaled up the true positives, false positives, true negatives, and false negatives.

Our learning set consisted of 13797 residues. In our test set, there were 198 assigned switches and 238 unassigned switches, for a total of 436 switches out of a total 2754 residues. We performed the logistic regression 6 times: twice on each of the switch types. Of each these two logistic regressions, one regression used the calculated E6, E20, and IsUnstruct values for the specific residue, whereas the other regression averaged E6, E20, and IsUnstruct values for each residue with its neighboring residues (but not Vkabat!) We label our tests as follows:

- **sa:** Single residue value, Assigned switches only
- **sb:** Single residue value, Both assigned and unassigned switches
- **su:** Single residue value, Unassigned switches only
- **ta:** Triplet residue value, Assigned switches only
- **tb:** Triplet residue value, Both assigned and unassigned switches
- **tu:** Triplet residue value, Unassigned switches only

For each descriptor combination in each regression, we plotted the true positive rate (TPR) against the false positive rate (FPR) (see Appendix B for fitting data) at thresholds of 0.01, and then we measured the AUC (Area Under the Curve). High AUC values correspond with a good descriptor combination. An AUC of 0.5 means the descriptor combination is essentially random when making predictions. We found that the accuracy of a prediction itself was not very useful, as the highest accuracies came almost exclusively from true negatives. We think this is because the signal is small compared to the background, since this is a similar problem to protein-protein interactions [22].

5.2 Which Descriptor Combinations Worked the Best?

Table 9: ROC AUC values for assigned+unassigned switches.

Descriptor Combination	Single residue value	Triplet residue value
E6 + IsU + VK	0.38588707443145387	0.3933273503732259
E6 + IsU	0.38187677608821274	0.39265451472718493
E6 + Res + IsU + VK	0.3841035652373527	0.3944889813268319
E6 + Res + IsU	0.3855600565181942	0.3933788025108643
E6 + Res + VK	0.4823751691983757	0.4790129698965416
E6 + Res	0.4820491407493014	0.47553203489246504
E6 + VK	0.4776455303923819	0.474197247706422
E6	0.4781412519492444	0.47597185172285505
E20 + IsU + VK	0.3905350824421559	0.39555760264701456
E20 + IsU	0.391089677118047	0.39598208278253166
E20 + Res + IsU + VK	0.3884290079236293	0.3970225043734316
E20 + Res + IsU	0.38738314427970966	0.3953948357885238
E20 + Res + VK	0.48421804624359815	0.48303415234582164
E20 + Res	0.48093005675566575	0.479067390426736
E20 + VK	0.4847360307446312	0.4790530431960484
E20	0.48068269070932707	0.47741102738045293
IsU + Res	0.3631575978975865	0.3630240202325637
IsU + VK	0.3654679967703889	0.3646858253318663
IsU	0.36700512938233687	0.3679085101835654
Res + IsU + VK	0.3635439836619674	0.3638739699677831
Res	0.4986889599544055	
VK + Res	0.5023014936951342	
VK	0.5295671687867587	

As one can see from Table 9, when trying to predict both types of switches, just about every descriptor combination fails miserably. Vkabat is the best at almost 0.53, but this is barely better than random. Lobanov-Galzitskaya's IsUnstruct when combined with the sequence performed the worst at around 0.36. Averaging the E6, E20, and IsUnstruct values over a residue and its neighbors caused only the most minimal change.

Table 10: ROC AUC values for assigned switches only.

Descriptor Combination	**Single residue value**	**Triplet residue value**
E6 + IsU + VK	0.5446473735792985	0.5300293624824142
E6 + IsU	0.4991207062803307	0.4779099682268696
E6 + Res + IsU + VK	0.5583900428383994	0.5501404894010528
E6 + Res + IsU	0.5144500561167228	0.5147889299884605
E6 + Res + VK	0.519042142868434	0.49978264649626153
E6 + Res	0.469330432652029	0.4578561435955802
E6 + VK	0.5178368188931569	0.5006332890722562
E6	0.4392546355574525	0.4261867501304121
E20 + IsU + VK	0.5387432620413841	0.5297280314885948
E20 + IsU	0.4688799181170073	0.48277473482872546
E20 + Res + IsU + VK	0.5499290637201436	0.5382700241855171
E20 + Res + IsU	0.5090537614011792	0.49887568960338924
E20 + Res + VK	0.5123545707465895	0.5044794581179557
E20 + Res	0.459464559523245	0.4468620081882993
E20 + VK	0.5176421887102638	0.4983332938145145
E20	0.43037080507737785	0.43857095999114776
IsU + Res	0.5615762476091115	0.5621374148369453
IsU + VK	0.5868356886549375	0.6002128088395694
IsU	0.6508571631811069	0.6590909090909092
Res + IsU + VK	0.5910345631589763	0.5886565182339831
Res	0.5115770379854887	
VK + Res	0.5635926953415217	
VK	0.6251491835412023	

When looking only at assigned switches, the AUC values appear to be better. However, entropy seems to be a bad predictor and residue type only does slightly better than random. Both IsUnstruct and Vkabat both seem fairly predictive, although triplet window averages do not seem to improve the results significantly. An unexpected result is that the IsUnstruct and Vkabat performed worse when combined than they did individually, but adding the qualitative descriptor RES (amino acid type) to the combination fared better than adding residues to the individual IsUnstruct and Vkabat.

Table 11: ROC AUC values for unassigned switches only.

Descriptor Combination	**Single residue value**	**Triplet residue value**
E6 + IsU + VK	0.44086752347998026	0.45158715314424663
E6 + IsU	0.43960084033613445	0.44734205287838513
E6 + Res + IsU + VK	0.4425149630599457	0.4503505297190419
E6 + Res + IsU	0.43506599778226074	0.44783052330630185
E6 + Res + VK	0.5045957969833402	0.5062891611334518
E6 + Res	0.5028807230364324	0.5069379500607875
E6 + VK	0.5076685682222014	0.5167299034081041
E6	0.5190920962979786	0.5162314130739736
E20 + IsU + VK	0.44434443093612636	0.4523553459539619
E20 + IsU	0.44468510774739156	0.4467341785680886
E20 + Res + IsU + VK	0.44539401611200913	0.45798653324604877
E20 + Res + IsU	0.4472927883395011	0.45407626484616104
E20 + Res + VK	0.5105325914149443	0.5195029124527395
E20 + Res	0.5066039531869981	0.516408431417082
E20 + VK	0.5168760270403869	0.530434630131862
E20	0.5178078783182589	0.5316854484242027
IsU + Res	0.42355730050366736	0.42392553205702
IsU + VK	0.431681774458591	0.43251175668995734
IsU	0.43278980908738696	0.4334636477802568
Res + IsU + VK	0.4354901738119731	0.4365982084407691
Res	0.5023120933588061	
VK + Res	0.505927609517575	
VK	0.5273084193931945	

Predicting unassigned switches also did not show much promise, with the best predictors doing only slightly better than random. It is notable, however, that we no longer see any values in the 0.3 to 0.4 range. Vkabat is once again the best.

CHAPTER 6

Discussion

Looking at the tables of AUC values, predicting for unassigned switched seemed fairly difficult. We suspect that this might be because many of the blanks in the DSSP files that correspond to unassigned switches might just be the result of missing data, and might not really be switches if they had known secondary structure data. The fact that all of the descriptors around the unassigned switches appear to be random supports this hypothesis. Furthermore, if this is true, it could help explain why the VKabat and IsUnstruct AUCs for assigned+unassigned switches compared to just the assigned switches is so low, since again, it is extremely likely that not all of the unassigned switches would actually be switches if we had all of the data.

We got the best results in terms of AUC when looking at switches with assigned secondary structure only. As one can see from Table 10, it did not make too much of a difference whether averaged entropy and IsUnstruct values over neighboring residues, so anything determined about the triplet-averaged values can probably be assumed for the single values also.

Among the descriptor combinations for assigned switches, three values stood out to us: IsUnstruct, Vkabat, and the combination of all four descriptors (using E6 for entropy). IsUnstruct gave us the best AUC value outright, but the ROC plot only had three unique points on the graph, out of the 100 different thresholds we plotted. This may also have something to do with the fact that the P value of the fit is surprisingly high, meaning that there is a very good change that a random

sample would give similar results, (see Table 12).

Table 12: Triplet Assigned: IsUnstruct.

	Beta	Standard Error	Z Value	$P > \|z\|$
Intercept	-2.2964	0.040	-57.098	0.000
IsUnstruct	-0.0216	0.123	-0.176	0.861

However, there is evidence that regions of disorder or regions that lend themselves to disorder under certain conditions may offer an additional alternative switch mechanism [23]. The Lobanov-Galzetskaya disorder propensity may be useful in computationally addressing the existence of such an alternative.

In a follow-up test, we made the threshold even thinner (0.001 instead of 0.01) and an additional point appeared on the graph, which brought the ROC value even higher, to 0.6939. The single residue version did even better, with an AUC of 0.6954. These values declined a little when we moved the threshold to 0.00001, resulting in values of 0.6808 (single) and 0.6805 (triplet). These values are consistent with the lower end of the AUC values for other sequence-based prediction studies of protein residues binding to RNA [24], which have AUC values of 0.68 to 0.78, where their adding homology-based data did significantly improve AUC values in some cases.

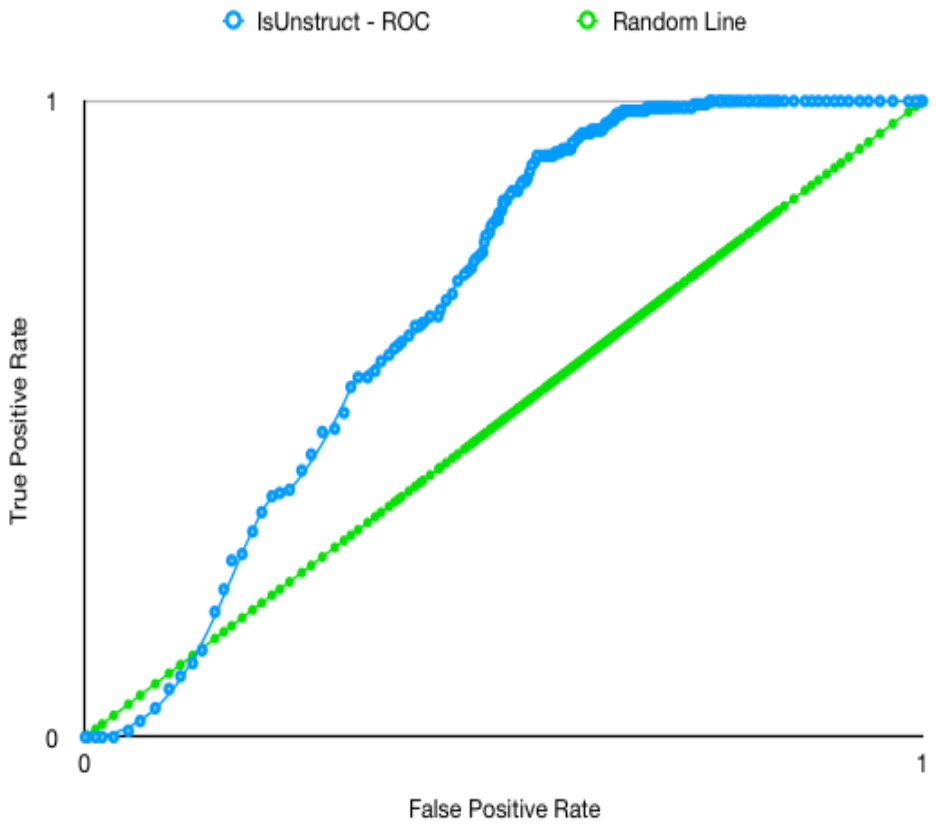


Figure 8: ROC plot of IsUnstruct at threshold of 0.00001.

The Vkabat from the Table 8 gave us almost as good an AUC value as IsUnstruct, and it does give us a much better fit with a much lower P-value. Unlike the IsUnstruct, the Vkabat ROC plot had 7 unique points (see Appendix C, Single/Assigned Vkabat), with somewhat even spacing, which lends support to the notion that the number of unique points and P-value are inversely correlated.

Table 13: Triplet Assigned: Vkabat.

	Beta	Standard Error	Z Value	$P > \|z\|$
Vkabat	0.0761	0.018	4.234	0.000
Intercept	-2.5291	0.063	-40.079	0.000

In a follow-up test, we made the threshold even thinner (0.001 instead of 0.01) see Figure 9, and another point appeared on the graph, which brought the AUC value down to 0.6365. Unlike with IsUnstruct, the AUC value did not change when the threshold was brought down to 0.00001 (also see Figure 9). This is because Vkabat values are discrete whereas the IsUnstruct are closer to continuous.

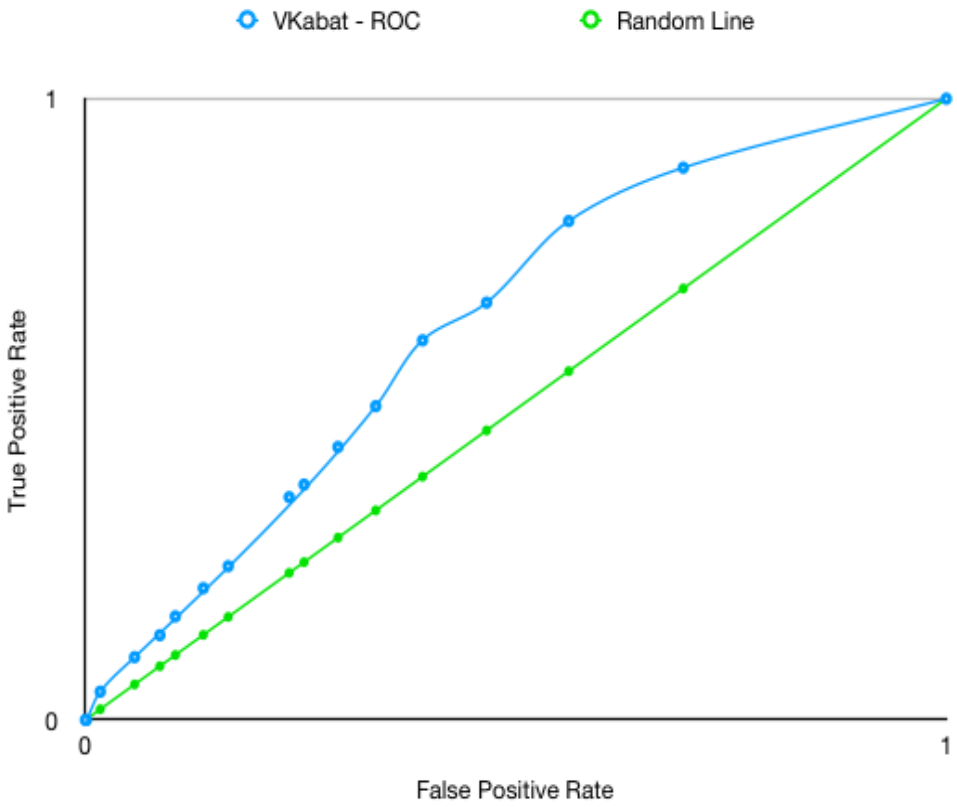


Figure 9: ROC plot of Vkabat at threshold of 0.00001.

The combination of all four descriptors (see Table 14) was interesting to us because it lets us look at all the descriptors side-by-side, including the qualitative descriptor.

Table 14: Triplet Assigned: Residue Type + E6 + IsUnstruct + Vkabat.

	Beta	Standard Error	Z Value	$P > \|z\|$
Intercept (Valine)	-2.9711	0.148	-20.022	0.000
Alanine	0.1699	0.172	0.990	0.322
Arginine	0.3294	0.179	1.837	0.066
Asparagine	0.3474	0.189	1.837	0.066
Aspartic Acid	0.4056	0.175	2.324	0.020
Cysteine	0.0942	0.317	0.297	0.766
Glutamine	0.5171	0.164	3.162	0.002
Glutamic acid	0.4653	0.185	2.511	0.012
Glycine	-0.3568	0.202	-1.765	0.078
Histidine	0.3064	0.220	1.391	0.164
Isoleucine	0.0837	0.185	0.453	0.650
Leucine	0.2121	0.160	1.323	0.186
Lysine	0.4416	0.170	2.593	0.010
Methionine	0.3012	0.240	1.254	0.210
Phenylalanine	0.4142	0.189	2.193	0.028
Proline	0.2646	0.202	1.310	0.190
Serine	0.3456	0.175	1.977	0.048
Threonine	0.0195	0.197	0.099	0.921
Tryptophan	0.5167	0.276	1.870	0.061
Tyrosine	0.2933	0.192	1.529	0.126
E6	0.4069	0.064	6.368	0
IsUnstruct	-0.1815	0.130	-1.398	0.162
Vkabat	0.0765	0.018	4.176	0.000

When we look at all four descriptors, the p-value for the IsUnstruct goes down significantly. However, this mainly applies to just the p-value for the IsUnstruct. As can be seen in Table 15, removing entropy from the calculation helps most of the P Values, (as well as increasing the AUC from 0.550 to 0.588). This time, the reducing the threshold caused the AUC values to stay pretty much the same at 0.548 (with E6) and 0.598 (without E6).

It's also interesting to note that the Vkabat p-value was not decreased when adding all of the other descriptors, and most of the other p-values are fairly small,

with a couple notable exceptions like threonine at 0.921.

Table 15: P - Values with and without entropy (E6).

Name	**P-value (E6)**	**P-value (No E6)**	**Difference**
Intercept (Valine)	0.000	0.000	0.000
Alanine	0.322	0.188	0.134
Arginine	0.066	0.030	0.036
Asparagine	0.066	0.033	0.033
Aspartic Acid	0.020	0.006	0.014
Cysteine	0.766	0.680	0.096
Glutamine	0.002	0.000	0.002
Glutamic acid	0.012	0.005	0.007
Glycine	0.078	0.126	-0.048
Histidine	0.164	0.107	0.057
Isoleucine	0.650	0.681	-0.031
Leucine	0.186	0.212	-0.026
Lysine	0.010	0.004	0.006
Methionine	0.210	0.099	0.111
Phenylalanine	0.028	0.028	0.000
Proline	0.190	0.108	0.082
Serine	0.048	0.020	0.028
Threonine	0.921	0.760	0.161
Tryptophan	0.061	0.074	-0.013
Tyrosine	0.126	0.144	-0.018
IsUnstruct	0.162	0.502	-0.340
Vkabat	0.000	0.000	0.000

As one can see from Table 15, IsUnstruct is a bit problematic. Where removing entropy usually caused an improvement in P-value (in fact, IsUnstruct is hurt the most by removing entropy). This is possibly related to the learning set being limited to the N-acetyltransferases which are themselves limited in number, and the test set being limited to the sirtuins which are even more limited in number.

6.1 Analyzing the Learning Set

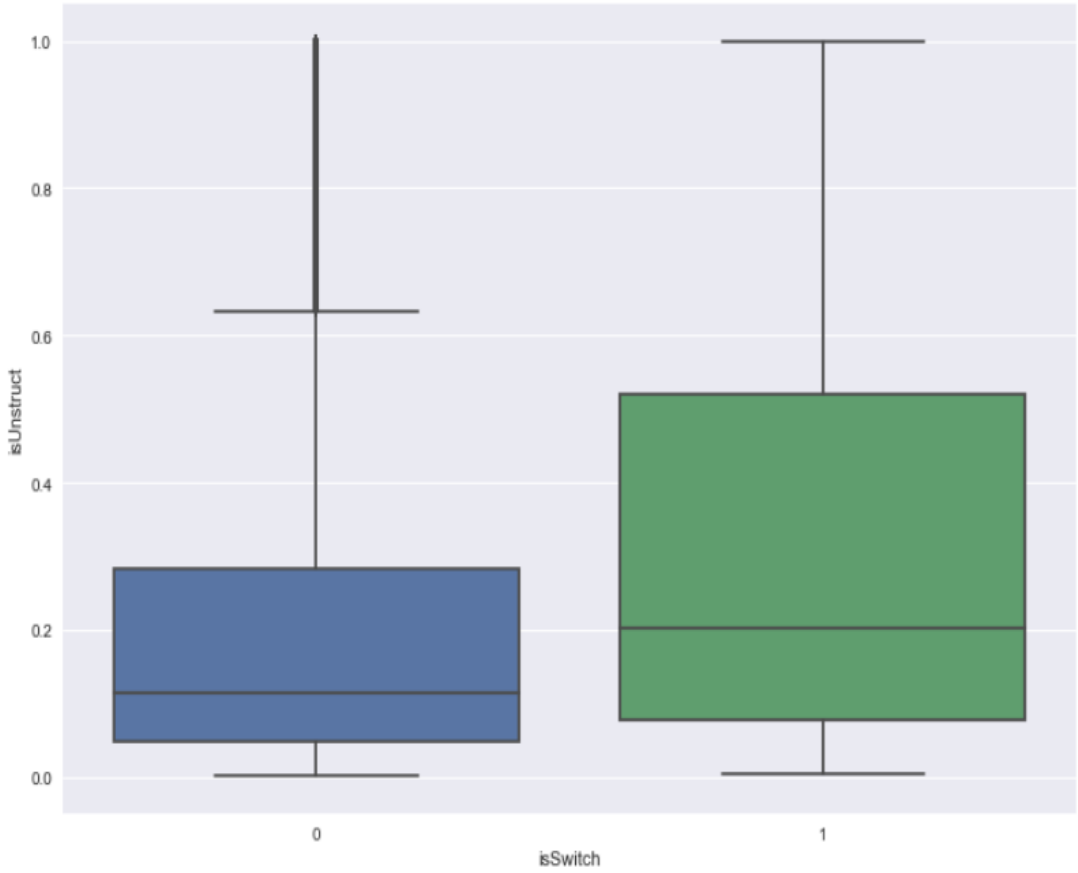


Figure 10: Histogram of IsUnstruct values from the Learning Set.
(Non-Switch: 0, Switch: 1).

However, as can be seen in Figure 10, the high p-value for the IsUnstruct alone is not enough to invalidate it as a potential decriptor. There is a significant differenence in the ranges of IsUnstruct values for switches and non-switches, whereas the E6 descriptor is less discriminating by itself, (see Figure 11).

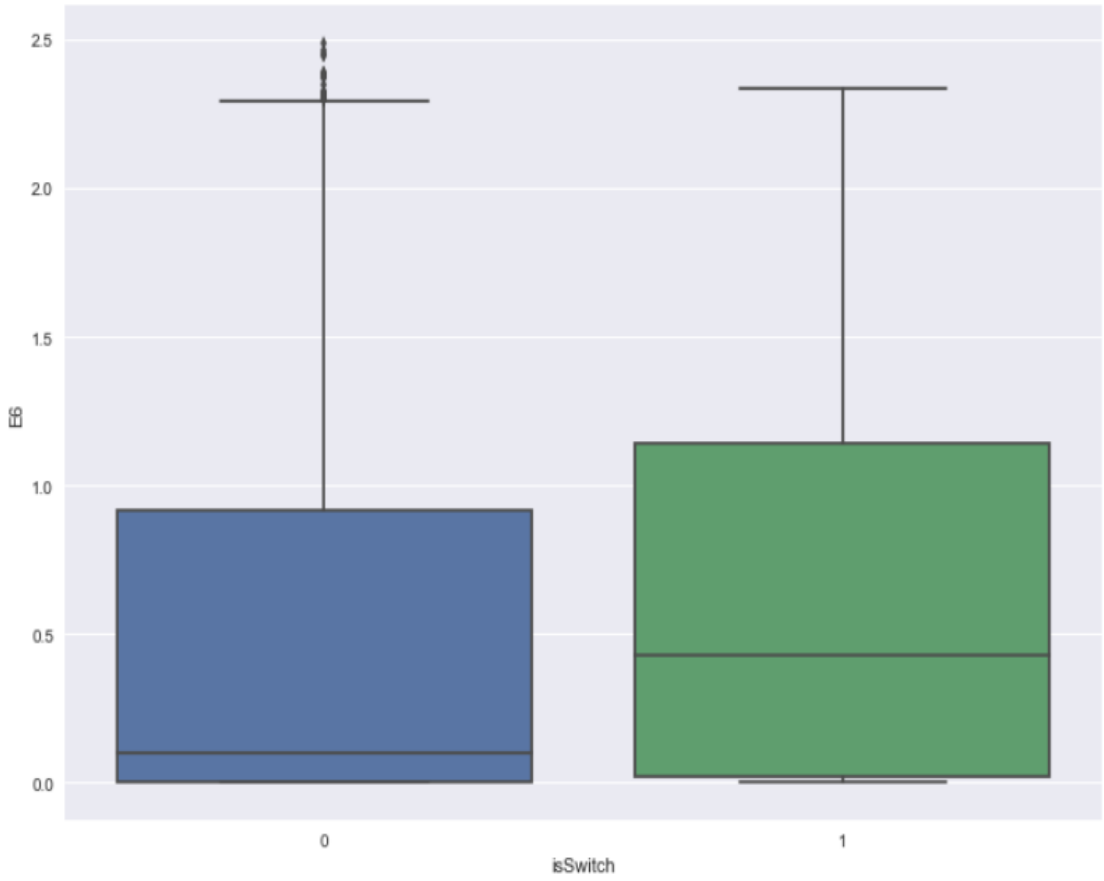


Figure 11: Histogram of E6 values from the Learning Set.
(Non-Switch: 0, Switch: 1).

6.1.1 Vkabat issues

Even though it proved to be predictive of the assigned switches, Vkabat proved to be a very difficult descriptor to use. The 15 algorithms that Vkabat uses vary drastically in their robustness, with many crashing at some times and completing at others, even on the same sequence. JPred in particular was very finicky when run via python script, as were PROF, SSPRO, YASPIN, JNET, and PsiPred, all of which were run through Sympred. MLRC crashed on 2REE:A, although it proved fairly robust most of the time.

We had previously tried Vkabat with GenBank sequences, and immediately ran into trouble since some of the algorithms that always crashed when fed a sequence with an 'X' residue. This, and the fact that some of the Sympred algorithms always crashed on certain sections of certain GenBank sequences, played a large part in why we eventually switched to Uniprot for our sequence data.

6.1.2 Entropy issues

Entropy never crashed on us in the same way as Vkabat, however entropy proposed its own set of issues. Specifically, the entropy values that we calculated changed over time. To determine entropy values (both 6-term and 20-term) we used a python script that calculated said values from a blast file. (We downloaded the blast files with other python scripts: either "getBlast.py" or "getBlastUniprot.py" depending on where the FASTA of the chain came from). However, our query sequences blast outputs change over time, likely as new proteins are added to the subject databases. An example of this is that, the blast file for 4JJX:A from January 19, 2019 is slightly different from the blast file for 4JJX:A from February 21, 2019. Thus, as more proteins get added to the protein databases, it is possible that entropy will become a better predictor of switch-like behavior, although the reverse may also be true.

6.2 Future Work

Like with many research projects, time constraints prevented us from doing everything desired. Specifically, there were other descriptors that we would have liked to look at and other learning and test sets to be considered.

In the area of test sets, we would have liked to have more clusters: specifically

at least around 100. It is possible that we may try something similar with all of the acetyltransferases in the future, and as more proteins get discovered, the number of N-acetyltransferases is bound to increase. Given the rarity of pyrrolysine and selenocysteine, the E22 is unlikely to make much of a difference, at least any time soon.

In and of itself, the DSSP cluster results (see Appendix D) are themselves interesting in describing possible switches for known x-ray and crystal structures and similarly interesting are the overlays of descriptor values (see Appendix E) for the same x-ray structures.

6.2.1 Residue Charge

Residue Charge is a descriptor that we also looked at, but did not have time to fully explore. The Java program is fully equipped to deal with charge, and uses two types of charge values, the Amber95 and the charges of various atoms within the residue [25], which is stored in a SQLite database included with the program. The charges in this database are not exact, but are the average charge for a residue type with a given secondary structure.

Aside from being averages, the charge database has some limitations: first, it only contains charge averages for the standard 20 amino acid residues. (If one asks the program it to assign a charge to a non-standard residue, the program will print a warning instead.). Second, it only contains the charges for the following backbone atoms and atom combinations: N, NH, O, C(alpha), C(beta), and C(prime), however, users can add other atoms to the residue using our addAtom() method. These atom charges are used to compute the value of averageCharge(), but not the value of amber95(), which is listed in the program's database.

We actually made two versions of the logistic regression script. The script "logistic-switch2.py" is the version we used for our calculation, but "logistic-switch3.py" is an advanced version that contains the ability to do a logistic regression on the amber95 as well as the descriptors in "logistic-switch2.py". It is not recommended to use "logistic-switch3.py" without modification, as doing a logistic regression on the amber95 causes the script to crash, as the values fail to converge. For anyone who can get this script to work, the output parser can also handle this, just set the boolean parameter of CSVParser.readFile() to true. All code is available upon request.

CHAPTER 7

Conclusions

The following are the most important results of this work. First, the clustering of possible secondary structure switches is, by itself, a useful algorithm, and the Logistic regression results suggest that prediction of switch-like behavior is doable. Based on ROC values alone, isUnstruct made the best prediction, in the case of assigned switches, however, the Vkabat consistently gave us better-than-average results, and was the best descriptor option overall. The overall trend of low-confidence ROC values may be because of the small size of the data set, a larger data set may give better results.

As stated in 6.2, residue charge may also be useful as a descriptor, and over time entropy may become a better descriptor as more proteins are catalogued, which will allow for better BLAST results.

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APPENDIX A

Complete Learning Set

Table A.16: Learning Set Clusters

Dominant Chain	**Other Chains**
1CJWA	1KUYA, 1KUXA, 1KUVA, 1IB1E, 1IB1F, 1IB1G, 1IB1H, 1B6BA, 1B6BB, 1L0CA
1GX3A	1GX3B, 1GX3C, 1GX3D, 1W6FC, 1W6FD, 1W6FA, 1W6FB, 1W5RA, 1W5RB
1IB1A	1iB1B, 1iB1C, 1iB1D, 4BG6A, 4BG6B, 3NKXA, 3NKXB, 3CU8A, 3CU8B, 2WH0A, 2WH0B, 2WH0C, 2WH0D, 1QJBA, 1QJBB, 1QJAA, 1QJAB, 1A4OA, 1A4OB, 1A4OC, 1A4OD, 1A38A, 1A38B, 1A37A, 1A37B, 5XY9A, 5XY9B, 5WXNA, 5WXNB, 5ULOA, 5ULOB, 4WRQA, 4WRQB, 4HKCA, 3RDHA, 3RDHB, 3RDHC, 3RDHD, 2V7DA, 2V7DB, 2V7DC, 2V7DD, 2C1NA, 2C1NB, 4ZDRA, 4ZDRB, 6FNCA, 6FNCB, 6FNBA, 6FNBB, 6FNAA, 6FNAB, 6FN9A, 6FN9B, 6F09P, 6F09Q, 6F09R, 6F09S, 6F08A, 6F08B, 6F08I, 6F08J, 6EWWA, 6EWWB, 6EWWC, 6EWWD, 6EJLA, 6EJLB, 5NASA, 5NASB, 5M37A, 5M37B, 5JM4A, 5JM4B, 5J31A, 5J31B, 5EXAA, 5EXAB, 5EWZA, 5EWZB, 5D3FA, 5D3FB, 5D2DA, 5D2DB, 4N7YA, 4N7YB, 4N7GA, 4IHLA, 4IHLB, 4FJ3A, 4FJ3B, 2O02A, 2O02B, 5M36A, 5M36B, 5M35A, 5M35B, 4N84A, 4N84B
1N71A	1N71B, 1N71C, 1N71D, 5E96A, 2A4NA, 2A4NB, 1B87A
1S7FA	1S7NA, 1S7NB, 1S7NC, 1S7ND, 1S7LA, 1S7KA, 1Z9UA, 1Z9UB
1TIQA	1TIQB
1XEBA	1XEBB, 1XEBC, 1XEBD, 1XEBE, 1XEBF, 1XEBG, 1XEBH,

2B5GA	2B5GB, 2B4DA, 2B4DB, 2B3UA, 2B3UB, 2B3VA, 2B4BA, 2B4BB, 2B58A, 2F5IA, 2F5IB, 2FXFA, 2FXFB, 2G3TA, 2G3TB, 2JEVA, 2JEVB, 3BJ7A, 3BJ7B, 3BJ7C, 3BJ7D, 3BJ8A, 3BJ8B, 3BJ8C, 3BJ8D
2BL1A	2J8MA, 2J8MB, 2J8NA, 2J8NB, 2J8RA, 2J8RB, 1YVOA, 1YVOB
2FIAA	2FIAB
2JLMA	2JLMB, 2JLMC, 2JLMD, 2JLME, 2JLMF
2Q4VA	2Q4VB, 2BEIA, 2BEIB
2REEA	2REEB, 2REFA, 2REFB
2VFBA	2VFCA, 2VFCB, 3LTWA, 4B55A, 4C5PA
2VI7A	2VI7B, 2VI7C
2WPWA	2WPWB, 2WPWC, 2WPWD, 2WPXA, 2WPXB
3FS8A	3FS8B, 3FSBA, 3FSBB, 3FSCA, 3FSCB
3MQHA	3MQHB, 3MQHC, 3MQHD, 3MQHE, 3MQHF
3N37A	4M1FA, 3N3BA, 3N3BB, 3N3AA, 3N3AB, 3N39A, 3N39B, 3N38A, 2R2FA, 2R2FB, 2BQ1I, 2BQ1J, 1R2FA, 1R2FB
3NE7A	3K9UA, 3K9UB, 3FIXA, 3FIXB, 3FIXC, 3FIXD, 3F0AA
3QB8A	3QB8B
3SMAA	3SMAB, 3SMAC, 3SMAD
3TFYA	3TFYB, 3TFYC, 4X5KA, 2PSWA, 2PSWB, 2PSWC, 2OB0A, 2OB0B, 2OB0C
3W6SA	3W6SB, 3W6SC, 3W91A, 3W91B, 3W91C, 3W6XA, 3W6XB, 3W6XC, 3W6XD, 3W6XE, 3W6XF, 3W6XG, 3W6XH, 3W6XI, 3W6XJ, 3W6XK, 3W6XL
4AVAA	4AVBA, 4AVBB, 4AVCA, 4AVCB
4EABA	4EAAA, 4EA9A, 4EA8A, 4EA7A
4FD4A	4FD4B, 5YAGA, 5YAGB
4FD5A	4FD6A
4FD7A	4FD7B, 4FD7C, 4FD7D
4HNYA	4HNYC, 4HNXA, 4HNWA, 4XPDA, 4XNHA, 4Y49A, 4Y49G, 4Y49M
4J3GA	4J3GB, 4J3GC, 4J3GD, 4JWPA, 4JWPB

4JJXA	4R57A, 4R57B, 4R57C, 4R57D, 4R57E, 4R57F, 4R57G, 4R57H, 4R57I, 4R57J, 4R57K, 4R57L, 4R87A, 4R87B, 4R87C, 4R87D, 4R87E, 4R87F, 4R87G, 4R87H, 4R87I, 4R87J, 4R87K, 4R87L, 4JJXB, 4JJXC, 4NCZA, 4NCZB, 4NCZC, 6CX8A, 6CX8B, 6CX8C, 6CX8D, 6CX8E, 6CX8F, 5CNPA, 5CNPB, 5CNPC, 5CNPD, 5CNPE, 5CNPF, 4MJ8A, 4MJ8B, 4MJ8C, 4JLYA, 4JLYB, 4JLYC, 4JLYD, 4JLYE, 4JLYF, 4MI4A, 4MI4B, 4MI4C, 4MHDA, 4MHDB, 4MHDC, 5UG4A, 5UG4B, 5UG4C, 4YGOA, 4YGOB, 4YGOC, 4YGOD, 4YGOE, 4YGOF, 6DAUA, 6DAUB, 6DAUC, 6DAUD, 6DAUE, 6DAUF
4KVOA	4KVOB, 4KVOC, 4KVOD, 4KVMA, 4KVMB, 4KVMC, 4KVMD
4KVXA	4KVXB
4PV6A	4PV6B, 4PV6C, 4PV6D, 4PV6E, 4PV6F, 4PV6G, 4PV6H, 4PV6I, 4PV6J, 4PV6K, 4PV6L, 4PV6M, 4PV6N, 4PV6O, 4PV6P
4R3KA	4R3LA, 5C88A, 5C88B, 4LX9A, 2X7BA
4R9MA	4R9MB, 4R9MC, 6CY6A, 3WR7A, 3WR7B, 3WR7C, 3WR7D
4RI1A	4RI1B, 4RI1C
4U9VB	4U9WA, 4U9WB, 4U9WC, 4U9WD
4UA3A	4UA3B
5GI5A	5GI8A, 5GI7A, 5GI6A, 3TE4A, 5GIHA, 5GIGA, 5GIFA, 5GIIA, 3V8IA, 3V8IB
5HGZA	5HH0A, 5HH1A, 5ICWA, 5ICWB, 5ICWC, 5ICWD
5JPHA	5JPHB, 5JPHC, 5JQ4A, 5JQ4B
5K04A	5K18A, 5K18C
5K9NA	5K9NB
5KTAA	5KTCA, 5KTDA
5WIFA	5WIFB, 5WIFC, 6D72A, 6D72B, 6D72C
5YGEA	5YGEB

APPENDIX B

Fitting Parameters

Of the following tables, all converged. All used the method of Maximum Likelihood Estimation (MLE), and all used the Logit model. Also, all had 13,797 observations

Table B.17: Fields: Single-Both: isSwitch - Residue Type

Field	**Value**
Accuracy:	84.17422867513612
Df Residuals:	13777
Df Model:	19
Date:	Thu Apr 04 16:28:39 PDT 2019
Pseudo R-squ.:	0.007754
Log-Likelihood:	-5294.1
LL-Null:	-5335.5
LLR p-value:	6.227E-10

Table B.18: Descriptors: Single-Both: isSwitch - Residue Type

Name	**Beta**	**Std Err**	**Z-score**	**P-value**
Intercept	-2.3695	0.118	-20.012	0.0
Alanine (A)	0.5033	0.15	3.364	0.001
Arginine (R)	0.4687	0.162	2.893	0.004
Asparagine (N)	0.6296	0.165	3.816	0.0
Aspartic acid (D)	0.7086	0.153	4.619	0.0
Cysteine (C)	0.3511	0.271	1.294	0.196
Glutamine (Q)	0.694	0.147	4.729	0.0
Glutamic acid (E)	0.6638	0.164	4.039	0.0
Glycine (G)	0.0567	0.168	0.338	0.735
Histidine (H)	0.43	0.199	2.165	0.03
Isoleucine (I)	0.175	0.167	1.051	0.293
Leucine (L)	0.3009	0.145	2.078	0.038
Lysine (K)	0.7615	0.149	5.099	0.0
Methionine (M)	0.7123	0.196	3.639	0.0
Phenylalanine (F)	0.395	0.175	2.261	0.024
Proline (P)	0.5331	0.173	3.083	0.002
Serine (S)	0.7323	0.151	4.843	0.0
Threonine (T)	0.3863	0.169	2.292	0.022
Tryptophan (W)	0.5283	0.254	2.082	0.037
Tyrosine (Y)	0.2635	0.177	1.49	0.136

Table B.19: Fields: Single-Both: isSwitch - E6

Field	**Value**
Accuracy:	84.17422867513612
Df Residuals:	13795
Df Model:	1
Date:	Thu Apr 04 16:28:39 PDT 2019
Pseudo R-squ.:	0.008374
Log-Likelihood:	-5290.8
LL-Null:	-5335.5
LLR p-value:	3.299E-21

Table B.20: Descriptors: Single-Both: isSwitch - E6

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.1035	0.034	-61.077	0.0
E6	0.3668	0.038	9.634	0.0

Table B.21: Fields: Single-Both: isSwitch - E20

Field	Value
Accuracy:	84.17422867513612
Df Residuals:	13795
Df Model:	1
Date:	Thu Apr 04 16:28:39 PDT 2019
Pseudo R-squ.:	0.01015
Log-Likelihood:	-5281.4
LL-Null:	-5335.5
LLR p-value:	2.316E-25

Table B.22: Descriptors: Single-Both: isSwitch - E20

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.1699	0.038	-57.488	0.0
E20	0.2902	0.027	10.566	0.0

Table B.23: Fields: Single-Both: isSwitch - isUnstruct

Field	Value
Accuracy:	84.17422867513612
Df Residuals:	13795
Df Model:	1
Date:	Thu Apr 04 16:28:39 PDT 2019
Pseudo R-squ.:	0.02014
Log-Likelihood:	-5228.1
LL-Null:	-5335.5
LLR p-value:	1.190E-48

Table B.24: Descriptors: Single-Both: isSwitch - isUnstruct

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.2459	0.036	-62.007	0.0
isUnstruct	1.3464	0.088	15.219	0.0

Table B.25: Fields: Single-Both: isSwitch - Vkabat

Field	Value
Accuracy:	84.17422867513612
Df Residuals:	13795
Df Model:	1
Date:	Thu Apr 04 16:28:39 PDT 2019
Pseudo R-squ.:	4.759E-5
Log-Likelihood:	-5335.3
LL-Null:	-5335.5
LLR p-value:	0.4761

Table B.26: Descriptors: Single-Both: isSwitch - Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-1.9329	0.053	-36.218	0.0
Vkabat	0.0113	0.016	0.714	0.475

Table B.27: Fields: Single-Both: isSwitch - E6 + Residue Type

Field	Value
Accuracy:	84.17422867513612
Df Residuals:	13776
Df Model:	20
Date:	Thu Apr 04 16:28:39 PDT 2019
Pseudo R-squ.:	0.01381
Log-Likelihood:	-5261.8
LL-Null:	-5335.5
LLR p-value:	1.985E-21

Table B.28: Descriptors: Single-Both: isSwitch - E6 + Residue Type

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.4724	0.119	-20.713	0.0
Alanine (A)	0.3772	0.151	2.502	0.012
Arginine (R)	0.3427	0.163	2.1	0.036
Asparagine (N)	0.508	0.166	3.058	0.002
Aspartic acid (D)	0.591	0.154	3.826	0.0
Cysteine (C)	0.2884	0.272	1.06	0.289
Glutamine (Q)	0.5658	0.148	3.824	0.0
Glutamic acid (E)	0.5013	0.166	3.02	0.003
Glycine (G)	-0.0344	0.168	-0.204	0.838
Histidine (H)	0.3112	0.2	1.559	0.119
Isoleucine (I)	0.1899	0.167	1.139	0.255
Leucine (L)	0.3179	0.145	2.192	0.028
Lysine (K)	0.6422	0.15	4.27	0.0
Methionine (M)	0.7326	0.196	3.737	0.0
Phenylalanine (F)	0.4019	0.175	2.298	0.022
Proline (P)	0.4207	0.174	2.419	0.016
Serine (S)	0.5848	0.153	3.831	0.0
Threonine (T)	0.2612	0.17	1.539	0.124
Tryptophan (W)	0.5648	0.254	2.222	0.026
Tyrosine (Y)	0.2754	0.177	1.555	0.12
E6	0.3282	0.04	8.148	0.0

Table B.29: Fields: Single-Both: isSwitch - E6 + isUnstruct

Field	Value
Accuracy:	84.17422867513612
Df Residuals:	13794
Df Model:	2
Date:	Thu Apr 04 16:28:40 PDT 2019
Pseudo R-squ.:	0.02588
Log-Likelihood:	-5197.5
LL-Null:	-5335.5
LLR p-value:	1.102E-60

Table B.30: Descriptors: Single-Both: isSwitch - E6 + isUnstruct

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.3979	0.042	-57.045	0.0
E6	0.3086	0.039	7.953	0.0
isUnstruct	1.269	0.09	14.165	0.0

Table B.31: Fields: Single-Both: isSwitch - E6 + Vkabat

Field	Value
Accuracy:	84.17422867513612
Df Residuals:	13794
Df Model:	2
Date:	Thu Apr 04 16:28:40 PDT 2019
Pseudo R-squ.:	0.008425
Log-Likelihood:	-5290.6
LL-Null:	-5335.5
LLR p-value:	3.011E-20

Table B.32: Descriptors: Single-Both: isSwitch - E6 + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.1381	0.058	-36.637	0.0
E6	0.3669	0.038	9.636	0.0
Vkabat	0.0117	0.016	0.738	0.46

Table B.33: Fields: Single-Both: isSwitch - E20 + Residue Type

Field	Value
Accuracy:	84.17422867513612
Df Residuals:	13776
Df Model:	20
Date:	Thu Apr 04 16:28:40 PDT 2019
Pseudo R-squ.:	0.01653
Log-Likelihood:	-5247.3
LL-Null:	-5335.5
LLR p-value:	4.912E-27

Table B.34: Descriptors: Single-Both: isSwitch - E20 + Residue Type

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.6412	0.122	-21.591	0.0
Alanine (A)	0.4919	0.15	3.279	0.001
Arginine (R)	0.4543	0.163	2.795	0.005
Asparagine (N)	0.6117	0.166	3.694	0.0
Aspartic acid (D)	0.6959	0.154	4.522	0.0
Cysteine (C)	0.3688	0.272	1.354	0.176
Glutamine (Q)	0.6796	0.147	4.617	0.0
Glutamic acid (E)	0.6251	0.165	3.79	0.0
Glycine (G)	0.1315	0.168	0.782	0.434
Histidine (H)	0.4237	0.199	2.126	0.033
Isoleucine (I)	0.1923	0.167	1.152	0.249
Leucine (L)	0.3913	0.145	2.69	0.007
Lysine (K)	0.7584	0.15	5.064	0.0
Methionine (M)	0.7564	0.196	3.851	0.0
Phenylalanine (F)	0.4979	0.175	2.838	0.005
Proline (P)	0.5783	0.174	3.333	0.001
Serine (S)	0.6833	0.152	4.502	0.0
Threonine (T)	0.3333	0.169	1.97	0.049
Tryptophan (W)	0.6982	0.255	2.738	0.006
Tyrosine (Y)	0.3698	0.178	2.082	0.037
E20	0.2754	0.028	9.801	0.0

Table B.35: Fields: Single-Both: isSwitch - E20 + isUnstruct

Field	Value
Accuracy:	84.17422867513612
Df Residuals:	13794
Df Model:	2
Date:	Thu Apr 04 16:28:40 PDT 2019
Pseudo R-squ.:	0.02789
Log-Likelihood:	-5186.7
LL-Null:	-5335.5
LLR p-value:	2.306E-65

Table B.36: Descriptors: Single-Both: isSwitch - E20 + isUnstruct

Name	**Beta**	**Std Err**	**Z-score**	**P-value**
Intercept	-2.4678	0.045	-54.901	0.0
E20	0.2571	0.028	9.224	0.0
isUnstruct	1.2768	0.09	14.265	0.0

Table B.37: Fields: Single-Both: isSwitch - E20 + Vkabat

Field	**Value**
Accuracy:	84.17422867513612
Df Residuals:	13794
Df Model:	2
Date:	Thu Apr 04 16:28:40 PDT 2019
Pseudo R-squ.:	0.01018
Log-Likelihood:	-5281.2
LL-Null:	-5335.5
LLR p-value:	2.625E-24

Table B.38: Descriptors: Single-Both: isSwitch - E20 + Vkabat

Name	**Beta**	**Std Err**	**Z-score**	**P-value**
Intercept	-2.1954	0.06	-36.595	0.0
E20	0.29	0.027	10.555	0.0
Vkabat	0.0087	0.016	0.548	0.584

Table B.39: Fields: Single-Both: isSwitch - isUnstruct + Vkabat

Field	**Value**
Accuracy:	84.17422867513612
Df Residuals:	13794
Df Model:	2
Date:	Thu Apr 04 16:28:40 PDT 2019
Pseudo R-squ.:	0.02056
Log-Likelihood:	-5225.8
LL-Null:	-5335.5
LLR p-value:	2.299E-48

Table B.40: Descriptors: Single-Both: isSwitch - isUnstruct + Vkabat

Name	**Beta**	**Std Err**	**Z-score**	**P-value**
Intercept	-2.3521	0.062	-37.927	0.0
isUnstruct	1.3659	0.089	15.355	0.0
Vkabat	0.0343	0.016	2.135	0.033

Table B.41: Fields: Single-Both: isSwitch - isUnstruct + Residue Type

Field	**Value**
Accuracy:	84.17422867513612
Df Residuals:	13776
Df Model:	20
Date:	Thu Apr 04 16:28:40 PDT 2019
Pseudo R-squ.:	0.02443
Log-Likelihood:	-5205.2
LL-Null:	-5335.5
LLR p-value:	7.954E-44

Table B.42: Descriptors: Single-Both: isSwitch - isUnstruct + Residue Type

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.6132	0.121	-21.664	0.0
Alanine (A)	0.4168	0.151	2.768	0.006
Arginine (R)	0.3482	0.163	2.133	0.033
Asparagine (N)	0.5423	0.166	3.262	0.001
Aspartic acid (D)	0.6069	0.155	3.928	0.0
Cysteine (C)	0.4216	0.272	1.547	0.122
Glutamine (Q)	0.5317	0.148	3.589	0.0
Glutamic acid (E)	0.4856	0.166	2.925	0.003
Glycine (G)	0.0192	0.168	0.114	0.909
Histidine (H)	0.4011	0.2	2.01	0.044
Isoleucine (I)	0.1914	0.167	1.144	0.253
Leucine (L)	0.289	0.145	1.986	0.047
Lysine (K)	0.5997	0.151	3.976	0.0
Methionine (M)	0.4432	0.199	2.226	0.026
Phenylalanine (F)	0.4813	0.176	2.743	0.006
Proline (P)	0.3109	0.175	1.777	0.076
Serine (S)	0.5072	0.153	3.31	0.001
Threonine (T)	0.2844	0.17	1.676	0.094
Tryptophan (W)	0.6513	0.255	2.556	0.011
Tyrosine (Y)	0.3533	0.178	1.989	0.047
isUnstruct	1.2749	0.093	13.764	0.0

Table B.43: Fields: Single-Both: isSwitch - Vkabat + Residue Type

Field	Value
Accuracy:	84.17422867513612
Df Residuals:	13776
Df Model:	20
Date:	Thu Apr 04 16:28:40 PDT 2019
Pseudo R-squ.:	0.007885
Log-Likelihood:	-5293.4
LL-Null:	-5335.5
LLR p-value:	7.690E-10

Table B.44: Descriptors: Single-Both: isSwitch - Vkabat + Residue Type

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.4315	0.13	-18.763	0.0
Alanine (A)	0.5122	0.15	3.419	0.001
Arginine (R)	0.469	0.162	2.895	0.004
Asparagine (N)	0.6389	0.165	3.867	0.0
Aspartic acid (D)	0.7175	0.154	4.671	0.0
Cysteine (C)	0.3526	0.271	1.299	0.194
Glutamine (Q)	0.7015	0.147	4.776	0.0
Glutamic acid (E)	0.6716	0.164	4.083	0.0
Glycine (G)	0.0689	0.168	0.41	0.682
Histidine (H)	0.4316	0.199	2.173	0.03
Isoleucine (I)	0.1742	0.167	1.046	0.295
Leucine (L)	0.3068	0.145	2.117	0.034
Lysine (K)	0.7688	0.149	5.144	0.0
Methionine (M)	0.7173	0.196	3.663	0.0
Phenylalanine (F)	0.3958	0.175	2.265	0.024
Proline (P)	0.5513	0.174	3.175	0.001
Serine (S)	0.737	0.151	4.872	0.0
Threonine (T)	0.3862	0.169	2.291	0.022
Tryptophan (W)	0.5261	0.254	2.073	0.038
Tyrosine (Y)	0.2655	0.177	1.501	0.133
Vkabat	0.0191	0.016	1.186	0.236

Table B.45: Fields: Single-Both: isSwitch - E6 + isUnstruct + Vkabat

Field	Value
Accuracy:	84.17422867513612
Df Residuals:	13793
Df Model:	3
Date:	Thu Apr 04 16:28:41 PDT 2019
Pseudo R-squ.:	0.02629
Log-Likelihood:	-5195.3
LL-Null:	-5335.5
LLR p-value:	1.646E-60

Table B.46: Descriptors: Single-Both: isSwitch - E6 + isUnstruct + Vkabat

Name	**Beta**	**Std Err**	**Z-score**	**P-value**
Intercept	-2.5027	0.066	-38.13	0.0
E6	0.3082	0.039	7.945	0.0
isUnstruct	1.2888	0.09	14.307	0.0
Vkabat	0.0339	0.016	2.105	0.035

Table B.47: Fields: Single-Both: isSwitch - E6 + Residue Type + Vkabat

Field	**Value**
Accuracy:	84.17422867513612
Df Residuals:	13775
Df Model:	21
Date:	Thu Apr 04 16:28:41 PDT 2019
Pseudo R-squ.:	0.01391
Log-Likelihood:	-5261.3
LL-Null:	-5335.5
LLR p-value:	3.454E-21

Table B.48: Descriptors: Single-Both: isSwitch - E6 + Residue Type + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.5268	0.131	-19.352	0.0
Alanine (A)	0.3857	0.151	2.555	0.011
Arginine (R)	0.344	0.163	2.108	0.035
Asparagine (N)	0.5167	0.166	3.106	0.002
Aspartic acid (D)	0.6001	0.155	3.879	0.0
Cysteine (C)	0.2906	0.272	1.068	0.285
Glutamine (Q)	0.5729	0.148	3.868	0.0
Glutamic acid (E)	0.5088	0.166	3.062	0.002
Glycine (G)	-0.0227	0.169	-0.135	0.893
Histidine (H)	0.3133	0.2	1.569	0.117
Isoleucine (I)	0.1896	0.167	1.137	0.256
Leucine (L)	0.3232	0.145	2.227	0.026
Lysine (K)	0.6495	0.151	4.314	0.0
Methionine (M)	0.7373	0.196	3.759	0.0
Phenylalanine (F)	0.403	0.175	2.304	0.021
Proline (P)	0.4374	0.175	2.504	0.012
Serine (S)	0.59	0.153	3.863	0.0
Threonine (T)	0.2622	0.17	1.545	0.122
Tryptophan (W)	0.5633	0.254	2.216	0.027
Tyrosine (Y)	0.2777	0.177	1.568	0.117
E6	0.3274	0.04	8.126	0.0
Vkabat	0.0167	0.016	1.034	0.301

Table B.49: Fields: Single-Both: isSwitch - E6 + Residue Type + isUnstruct

Field	Value
Accuracy:	84.17422867513612
Df Residuals:	13775
Df Model:	21
Date:	Thu Apr 04 16:28:41 PDT 2019
Pseudo R-squ.:	0.02943
Log-Likelihood:	-5178.5
LL-Null:	-5335.5
LLR p-value:	4.424E-54

Table B.50: Descriptors: Single-Both: isSwitch - E6 + Residue Type + isUnstruct

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.7025	0.122	-22.23	0.0
Alanine (A)	0.3024	0.152	1.993	0.046
Arginine (R)	0.2374	0.164	1.445	0.149
Asparagine (N)	0.4324	0.167	2.583	0.01
Aspartic acid (D)	0.5046	0.155	3.246	0.001
Cysteine (C)	0.3608	0.273	1.32	0.187
Glutamine (Q)	0.4228	0.149	2.835	0.005
Glutamic acid (E)	0.3498	0.167	2.091	0.037
Glycine (G)	-0.0675	0.169	-0.399	0.69
Histidine (H)	0.2932	0.201	1.461	0.144
Isoleucine (I)	0.2051	0.168	1.224	0.221
Leucine (L)	0.3055	0.146	2.097	0.036
Lysine (K)	0.4987	0.152	3.286	0.001
Methionine (M)	0.4785	0.199	2.404	0.016
Phenylalanine (F)	0.4854	0.176	2.762	0.006
Proline (P)	0.2128	0.176	1.209	0.227
Serine (S)	0.3749	0.155	2.423	0.015
Threonine (T)	0.175	0.171	1.025	0.305
Tryptophan (W)	0.6847	0.255	2.685	0.007
Tyrosine (Y)	0.3627	0.178	2.039	0.041
E6	0.3015	0.041	7.394	0.0
isUnstruct	1.2391	0.093	13.31	0.0

Table B.51: Fields: Single-Both: isSwitch - E20 + isUnstruct + Vkabat

Field	Value
Accuracy:	84.17422867513612
Df Residuals:	13793
Df Model:	3
Date:	Thu Apr 04 16:28:41 PDT 2019
Pseudo R-squ.:	0.02823
Log-Likelihood:	-5184.9
LL-Null:	-5335.5
LLR p-value:	5.239E-65

Table B.52: Descriptors: Single-Both: isSwitch - E20 + isUnstruct + Vkabat

Name	**Beta**	**Std Err**	**Z-score**	**P-value**
Intercept	-2.562	0.067	-38.181	0.0
E20	0.2557	0.028	9.173	0.0
isUnstruct	1.2947	0.09	14.386	0.0
Vkabat	0.0308	0.016	1.911	0.056

Table B.53: Fields: Single-Both: isSwitch - E20 + Residue Type + Vkabat

Field	**Value**
Accuracy:	84.17422867513612
Df Residuals:	13775
Df Model:	21
Date:	Thu Apr 04 16:28:41 PDT 2019
Pseudo R-squ.:	0.01663
Log-Likelihood:	-5246.8
LL-Null:	-5335.5
LLR p-value:	9.239E-27

Table B.54: Descriptors: Single-Both: isSwitch - E20 + Residue Type + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.6951	0.133	-20.247	0.0
Alanine (A)	0.4997	0.15	3.326	0.001
Arginine (R)	0.4551	0.163	2.799	0.005
Asparagine (N)	0.6197	0.166	3.738	0.0
Aspartic acid (D)	0.7045	0.154	4.571	0.0
Cysteine (C)	0.3706	0.272	1.361	0.174
Glutamine (Q)	0.6861	0.147	4.657	0.0
Glutamic acid (E)	0.6319	0.165	3.827	0.0
Glycine (G)	0.1426	0.169	0.846	0.398
Histidine (H)	0.4253	0.199	2.134	0.033
Isoleucine (I)	0.1916	0.167	1.148	0.251
Leucine (L)	0.3962	0.146	2.722	0.006
Lysine (K)	0.7652	0.15	5.103	0.0
Methionine (M)	0.7609	0.196	3.873	0.0
Phenylalanine (F)	0.4986	0.175	2.842	0.004
Proline (P)	0.5943	0.174	3.411	0.001
Serine (S)	0.688	0.152	4.531	0.0
Threonine (T)	0.3337	0.169	1.972	0.049
Tryptophan (W)	0.6963	0.255	2.73	0.006
Tyrosine (Y)	0.3716	0.178	2.092	0.036
E20	0.2748	0.028	9.783	0.0
Vkabat	0.0167	0.016	1.034	0.301

Table B.55: Fields: Single-Both: isSwitch - E20 + Residue Type + isUnstruct

Field	Value
Accuracy:	84.17422867513612
Df Residuals:	13775
Df Model:	21
Date:	Thu Apr 04 16:28:41 PDT 2019
Pseudo R-squ.:	0.03192
Log-Likelihood:	-5165.2
LL-Null:	-5335.5
LLR p-value:	1.570E-59

Table B.56: Descriptors: Single-Both: isSwitch - E20 + Residue Type + isUnstruct

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.8593	0.124	-22.987	0.0
Alanine (A)	0.4063	0.151	2.691	0.007
Arginine (R)	0.3378	0.164	2.063	0.039
Asparagine (N)	0.5255	0.167	3.149	0.002
Aspartic acid (D)	0.5987	0.155	3.865	0.0
Cysteine (C)	0.4343	0.274	1.588	0.112
Glutamine (Q)	0.5271	0.148	3.55	0.0
Glutamic acid (E)	0.4641	0.166	2.79	0.005
Glycine (G)	0.084	0.169	0.497	0.619
Histidine (H)	0.3939	0.2	1.966	0.049
Isoleucine (I)	0.2049	0.168	1.222	0.222
Leucine (L)	0.3726	0.146	2.55	0.011
Lysine (K)	0.6052	0.151	4.003	0.0
Methionine (M)	0.5087	0.199	2.556	0.011
Phenylalanine (F)	0.5742	0.176	3.258	0.001
Proline (P)	0.3586	0.176	2.042	0.041
Serine (S)	0.4639	0.154	3.015	0.003
Threonine (T)	0.2387	0.17	1.402	0.161
Tryptophan (W)	0.8087	0.256	3.161	0.002
Tyrosine (Y)	0.4494	0.178	2.52	0.012
E20	0.2572	0.028	9.05	0.0
isUnstruct	1.2325	0.093	13.213	0.0

Table B.57: Fields: Single-Both: isSwitch - Residue Type + isUnstruct + Vkabat

Field	Value
Accuracy:	84.17422867513612
Df Residuals:	13775
Df Model:	21
Date:	Thu Apr 04 16:28:42 PDT 2019
Pseudo R-squ.:	0.02493
Log-Likelihood:	-5202.5
LL-Null:	-5335.5
LLR p-value:	2.494E-44

Table B.58: Descriptors: Single-Both: isSwitch - Residue Type + isUnstruct + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.7415	0.133	-20.587	0.0
Alanine (A)	0.435	0.151	2.884	0.004
Arginine (R)	0.3484	0.163	2.134	0.033
Asparagine (N)	0.5629	0.167	3.38	0.001
Aspartic acid (D)	0.6261	0.155	4.045	0.0
Cysteine (C)	0.4286	0.273	1.573	0.116
Glutamine (Q)	0.547	0.148	3.688	0.0
Glutamic acid (E)	0.502	0.166	3.02	0.003
Glycine (G)	0.0469	0.169	0.277	0.781
Histidine (H)	0.4068	0.2	2.038	0.042
Isoleucine (I)	0.19	0.167	1.135	0.256
Leucine (L)	0.3016	0.146	2.07	0.038
Lysine (K)	0.6138	0.151	4.064	0.0
Methionine (M)	0.4514	0.199	2.266	0.023
Phenylalanine (F)	0.4857	0.176	2.766	0.006
Proline (P)	0.3465	0.176	1.972	0.049
Serine (S)	0.5168	0.153	3.371	0.001
Threonine (T)	0.2851	0.17	1.679	0.093
Tryptophan (W)	0.6504	0.255	2.552	0.011
Tyrosine (Y)	0.3599	0.178	2.025	0.043
isUnstruct	1.2935	0.093	13.915	0.0
Vkabat	0.0377	0.016	2.314	0.021

Table B.59: Fields: Single-Both: isSwitch - E6 + Residue Type + isUnstruct + Vkabat

Field	Value
Accuracy:	84.17422867513612
Df Residuals:	13774
Df Model:	22
Date:	Thu Apr 04 16:28:42 PDT 2019
Pseudo R-squ.:	0.02986
Log-Likelihood:	-5176.2
LL-Null:	-5335.5
LLR p-value:	2.043E-54

Table B.60: Descriptors: Single-Both: isSwitch - E6 + Residue Type + isUnstruct + Vkabat

Name	**Beta**	**Std Err**	**Z-score**	**P-value**
Intercept	-2.8219	0.134	-21.046	0.0
Alanine (A)	0.3209	0.152	2.11	0.035
Arginine (R)	0.2395	0.164	1.457	0.145
Asparagine (N)	0.4527	0.168	2.7	0.007
Aspartic acid (D)	0.5249	0.156	3.37	0.001
Cysteine (C)	0.3689	0.273	1.35	0.177
Glutamine (Q)	0.438	0.149	2.932	0.003
Glutamic acid (E)	0.3664	0.168	2.187	0.029
Glycine (G)	-0.0398	0.17	-0.234	0.815
Histidine (H)	0.2997	0.201	1.493	0.135
Isoleucine (I)	0.2045	0.168	1.22	0.222
Leucine (L)	0.3175	0.146	2.176	0.03
Lysine (K)	0.5136	0.152	3.38	0.001
Methionine (M)	0.4864	0.199	2.443	0.015
Phenylalanine (F)	0.4902	0.176	2.788	0.005
Proline (P)	0.2473	0.177	1.399	0.162
Serine (S)	0.3858	0.155	2.492	0.013
Threonine (T)	0.1777	0.171	1.041	0.298
Tryptophan (W)	0.6846	0.255	2.684	0.007
Tyrosine (Y)	0.3699	0.178	2.078	0.038
E6	0.2994	0.041	7.342	0.0
isUnstruct	1.2568	0.093	13.45	0.0
Vkabat	0.0351	0.016	2.147	0.032

Table B.61: Fields: Single-Both: isSwitch - E20 + Residue Type + isUnstruct + Vkabat

Field	**Value**
Accuracy:	84.17422867513612
Df Residuals:	13774
Df Model:	22
Date:	Thu Apr 04 16:28:42 PDT 2019
Pseudo R-squ.:	0.03234
Log-Likelihood:	-5163.0
LL-Null:	-5335.5
LLR p-value:	7.783E-60

Table B.62: Descriptors: Single-Both: isSwitch - E20 + Residue Type + isUnstruct + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.9764	0.136	-21.816	0.0
Alanine (A)	0.4231	0.151	2.797	0.005
Arginine (R)	0.339	0.164	2.07	0.038
Asparagine (N)	0.5442	0.167	3.256	0.001
Aspartic acid (D)	0.6178	0.155	3.98	0.0
Cysteine (C)	0.4415	0.274	1.614	0.107
Glutamine (Q)	0.5409	0.149	3.639	0.0
Glutamic acid (E)	0.479	0.167	2.876	0.004
Glycine (G)	0.1101	0.17	0.649	0.516
Histidine (H)	0.3994	0.2	1.993	0.046
Isoleucine (I)	0.2038	0.168	1.215	0.224
Leucine (L)	0.3837	0.146	2.623	0.009
Lysine (K)	0.6188	0.151	4.088	0.0
Methionine (M)	0.5163	0.199	2.593	0.01
Phenylalanine (F)	0.578	0.176	3.279	0.001
Proline (P)	0.3914	0.176	2.22	0.026
Serine (S)	0.4737	0.154	3.077	0.002
Threonine (T)	0.2403	0.17	1.411	0.158
Tryptophan (W)	0.8076	0.256	3.156	0.002
Tyrosine (Y)	0.4557	0.178	2.554	0.011
E20	0.2559	0.028	9.003	0.0
isUnstruct	1.2499	0.094	13.351	0.0
Vkabat	0.0348	0.016	2.126	0.033

Table B.63: Fields: Single-Assigned: isSwitch - Residue Type

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13777
Df Model:	19
Date:	Thu Apr 04 16:28:32 PDT 2019
Pseudo R-squ.:	0.005799
Log-Likelihood:	-4187.2
LL-Null:	-4211.6
LLR p-value:	0.0001935

Table B.64: Descriptors: Single-Assigned: isSwitch - Residue Type

Name	**Beta**	**Std Err**	**Z-score**	**P-value**
Intercept	-2.5673	0.129	-19.947	0.0
Alanine (A)	0.1842	0.171	1.079	0.281
Arginine (R)	0.3808	0.178	2.135	0.033
Asparagine (N)	0.3589	0.188	1.908	0.056
Aspartic acid (D)	0.4351	0.173	2.51	0.012
Cysteine (C)	0.1283	0.317	0.405	0.685
Glutamine (Q)	0.5342	0.162	3.293	0.001
Glutamic acid (E)	0.4745	0.184	2.579	0.01
Glycine (G)	-0.3602	0.201	-1.79	0.073
Histidine (H)	0.345	0.22	1.571	0.116
Isoleucine (I)	0.0797	0.184	0.432	0.666
Leucine (L)	0.1754	0.16	1.097	0.273
Lysine (K)	0.4458	0.169	2.636	0.008
Methionine (M)	0.3481	0.231	1.505	0.132
Phenylalanine (F)	0.4163	0.188	2.21	0.027
Proline (P)	0.2354	0.2	1.178	0.239
Serine (S)	0.3714	0.173	2.146	0.032
Threonine (T)	0.0556	0.197	0.283	0.777
Tryptophan (W)	0.5078	0.276	1.843	0.065
Tyrosine (Y)	0.2757	0.191	1.441	0.149

Table B.65: Fields: Single-Assigned: isSwitch - E6

Field	**Value**
Accuracy:	92.8130671506352
Df Residuals:	13795
Df Model:	1
Date:	Thu Apr 04 16:28:33 PDT 2019
Pseudo R-squ.:	0.003655
Log-Likelihood:	-4196.2
LL-Null:	-4211.6
LLR p-value:	2.881E-8

Table B.66: Descriptors: Single-Assigned: isSwitch - E6

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.4374	0.04	-61.482	0.0
E6	0.2538	0.045	5.645	0.0

Table B.67: Fields: Single-Assigned: isSwitch - E20

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13795
Df Model:	1
Date:	Thu Apr 04 16:28:33 PDT 2019
Pseudo R-squ.:	0.004762
Log-Likelihood:	-4191.6
LL-Null:	-4211.6
LLR p-value:	2.396E-10

Table B.68: Descriptors: Single-Assigned: isSwitch - E20

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.4893	0.043	-57.353	0.0
E20	0.2077	0.032	6.43	0.0

Table B.69: Fields: Single-Assigned: isSwitch - isUnstruct

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13795
Df Model:	1
Date:	Thu Apr 04 16:28:33 PDT 2019
Pseudo R-squ.:	5.824E-6
Log-Likelihood:	-4211.6
LL-Null:	-4211.6
LLR p-value:	0.8247

Table B.70: Descriptors: Single-Assigned: isSwitch - isUnstruct

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.2934	0.04	-57.469	0.0
isUnstruct	-0.0265	0.12	-0.221	0.825

Table B.71: Fields: Single-Assigned: isSwitch - Vkabat

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13795
Df Model:	1
Date:	Thu Apr 04 16:28:33 PDT 2019
Pseudo R-squ.:	0.00208
Log-Likelihood:	-4202.9
LL-Null:	-4211.6
LLR p-value:	0.00002848

Table B.72: Descriptors: Single-Assigned: isSwitch - Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.5291	0.063	-40.079	0.0
Vkabat	0.0761	0.018	4.234	0.0

Table B.73: Fields: Single-Assigned: isSwitch - E6 + Residue Type

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13776
Df Model:	20
Date:	Thu Apr 04 16:28:33 PDT 2019
Pseudo R-squ.:	0.008831
Log-Likelihood:	-4174.4
LL-Null:	-4211.6
LLR p-value:	3.452E-8

Table B.74: Descriptors: Single-Assigned: isSwitch - E6 + Residue Type

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.6418	0.13	-20.363	0.0
Alanine (A)	0.0906	0.172	0.527	0.598
Arginine (R)	0.2885	0.18	1.607	0.108
Asparagine (N)	0.2686	0.189	1.42	0.156
Aspartic acid (D)	0.3475	0.174	1.993	0.046
Cysteine (C)	0.0818	0.317	0.258	0.796
Glutamine (Q)	0.4393	0.164	2.687	0.007
Glutamic acid (E)	0.3542	0.186	1.907	0.057
Glycine (G)	-0.4272	0.202	-2.116	0.034
Histidine (H)	0.258	0.221	1.169	0.242
Isoleucine (I)	0.0903	0.185	0.489	0.625
Leucine (L)	0.1873	0.16	1.17	0.242
Lysine (K)	0.3568	0.17	2.095	0.036
Methionine (M)	0.3619	0.231	1.563	0.118
Phenylalanine (F)	0.4208	0.188	2.233	0.026
Proline (P)	0.1521	0.201	0.758	0.449
Serine (S)	0.2614	0.175	1.497	0.134
Threonine (T)	-0.0371	0.198	-0.188	0.851
Tryptophan (W)	0.5341	0.276	1.937	0.053
Tyrosine (Y)	0.2842	0.191	1.485	0.138
E6	0.2435	0.048	5.12	0.0

Table B.75: Fields: Single-Assigned: isSwitch - E6 + isUnstruct

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13794
Df Model:	2
Date:	Thu Apr 04 16:28:33 PDT 2019
Pseudo R-squ.:	0.003754
Log-Likelihood:	-4195.8
LL-Null:	-4211.6
LLR p-value:	1.360E-7

Table B.76: Descriptors: Single-Assigned: isSwitch - E6 + isUnstruct

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.4154	0.046	-52.198	0.0
E6	0.259	0.045	5.718	0.0
isUnstruct	-0.1105	0.122	-0.908	0.364

Table B.77: Fields: Single-Assigned: isSwitch - E6 + Vkabat

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13794
Df Model:	2
Date:	Thu Apr 04 16:28:33 PDT 2019
Pseudo R-squ.:	0.005747
Log-Likelihood:	-4187.4
LL-Null:	-4211.6
LLR p-value:	3.075E-11

Table B.78: Descriptors: Single-Assigned: isSwitch - E6 + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.6681	0.068	-38.974	0.0
E6	0.2544	0.045	5.655	0.0
Vkabat	0.0764	0.018	4.247	0.0

Table B.79: Fields: Single-Assigned: isSwitch - E20 + Residue Type

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13776
Df Model:	20
Date:	Thu Apr 04 16:28:33 PDT 2019
Pseudo R-squ.:	0.01016
Log-Likelihood:	-4168.8
LL-Null:	-4211.6
LLR p-value:	4.287E-10

Table B.80: Descriptors: Single-Assigned: isSwitch - E20 + Residue Type

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.764	0.133	-20.751	0.0
Alanine (A)	0.1748	0.171	1.023	0.306
Arginine (R)	0.3707	0.179	2.076	0.038
Asparagine (N)	0.3448	0.188	1.83	0.067
Aspartic acid (D)	0.4243	0.174	2.445	0.015
Cysteine (C)	0.1413	0.317	0.446	0.656
Glutamine (Q)	0.5228	0.162	3.219	0.001
Glutamic acid (E)	0.4455	0.184	2.417	0.016
Glycine (G)	-0.3057	0.202	-1.516	0.129
Histidine (H)	0.3407	0.22	1.549	0.121
Isoleucine (I)	0.0917	0.185	0.496	0.62
Leucine (L)	0.2409	0.16	1.501	0.133
Lysine (K)	0.4419	0.169	2.609	0.009
Methionine (M)	0.3786	0.232	1.634	0.102
Phenylalanine (F)	0.4911	0.189	2.598	0.009
Proline (P)	0.2676	0.2	1.337	0.181
Serine (S)	0.3336	0.173	1.924	0.054
Threonine (T)	0.0163	0.197	0.083	0.934
Tryptophan (W)	0.6314	0.277	2.283	0.022
Tyrosine (Y)	0.3532	0.192	1.841	0.066
E20	0.203	0.033	6.144	0.0

Table B.81: Fields: Single-Assigned: isSwitch - E20 + isUnstruct

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13794
Df Model:	2
Date:	Thu Apr 04 16:28:34 PDT 2019
Pseudo R-squ.:	0.004852
Log-Likelihood:	-4191.2
LL-Null:	-4211.6
LLR p-value:	1.333E-9

Table B.82: Descriptors: Single-Assigned: isSwitch - E20 + isUnstruct

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.4684	0.05	-49.849	0.0
E20	0.2106	0.032	6.487	0.0
isUnstruct	-0.1052	0.121	-0.866	0.386

Table B.83: Fields: Single-Assigned: isSwitch - E20 + Vkabat

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13794
Df Model:	2
Date:	Thu Apr 04 16:28:34 PDT 2019
Pseudo R-squ.:	0.006747
Log-Likelihood:	-4183.2
LL-Null:	-4211.6
LLR p-value:	4.555E-13

Table B.84: Descriptors: Single-Assigned: isSwitch - E20 + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.7119	0.07	-38.585	0.0
E20	0.2055	0.032	6.365	0.0
Vkabat	0.0744	0.018	4.136	0.0

Table B.85: Fields: Single-Assigned: isSwitch - isUnstruct + Vkabat

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13794
Df Model:	2
Date:	Thu Apr 04 16:28:34 PDT 2019
Pseudo R-squ.:	0.002083
Log-Likelihood:	-4202.9
LL-Null:	-4211.6
LLR p-value:	0.0001549

Table B.86: Descriptors: Single-Assigned: isSwitch - isUnstruct + Vkabat

Name	**Beta**	**Std Err**	**Z-score**	**P-value**
Intercept	-2.5346	0.071	-35.774	0.0
isUnstruct	0.0205	0.12	0.17	0.865
Vkabat	0.0764	0.018	4.231	0.0

Table B.87: Fields: Single-Assigned: isSwitch - isUnstruct + Residue Type

Field	**Value**
Accuracy:	92.8130671506352
Df Residuals:	13776
Df Model:	20
Date:	Thu Apr 04 16:28:34 PDT 2019
Pseudo R-squ.:	0.005926
Log-Likelihood:	-4186.7
LL-Null:	-4211.6
LLR p-value:	0.0002276

Table B.88: Descriptors: Single-Assigned: isSwitch - isUnstruct + Residue Type

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.5463	0.13	-19.545	0.0
Alanine (A)	0.1924	0.171	1.126	0.26
Arginine (R)	0.3923	0.179	2.195	0.028
Asparagine (N)	0.367	0.188	1.949	0.051
Aspartic acid (D)	0.4452	0.174	2.564	0.01
Cysteine (C)	0.1226	0.317	0.387	0.699
Glutamine (Q)	0.5496	0.163	3.374	0.001
Glutamic acid (E)	0.4913	0.185	2.66	0.008
Glycine (G)	-0.3567	0.201	-1.772	0.076
Histidine (H)	0.3485	0.22	1.586	0.113
Isoleucine (I)	0.0785	0.184	0.426	0.67
Leucine (L)	0.1769	0.16	1.106	0.269
Lysine (K)	0.4609	0.17	2.715	0.007
Methionine (M)	0.3718	0.232	1.599	0.11
Phenylalanine (F)	0.4095	0.188	2.172	0.03
Proline (P)	0.2559	0.201	1.275	0.202
Serine (S)	0.3925	0.174	2.252	0.024
Threonine (T)	0.065	0.197	0.33	0.741
Tryptophan (W)	0.4977	0.276	1.805	0.071
Tyrosine (Y)	0.2685	0.191	1.403	0.161
isUnstruct	-0.1288	0.125	-1.029	0.303

Table B.89: Fields: Single-Assigned: isSwitch - Vkabat + Residue Type

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13776
Df Model:	20
Date:	Thu Apr 04 16:28:34 PDT 2019
Pseudo R-squ.:	0.007938
Log-Likelihood:	-4178.2
LL-Null:	-4211.6
LLR p-value:	5.877E-7

Table B.90: Descriptors: Single-Assigned: isSwitch - Vkabat + Residue Type

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.8271	0.143	-19.762	0.0
Alanine (A)	0.221	0.171	1.292	0.196
Arginine (R)	0.3823	0.178	2.142	0.032
Asparagine (N)	0.3988	0.188	2.116	0.034
Aspartic acid (D)	0.4737	0.174	2.727	0.006
Cysteine (C)	0.1348	0.317	0.426	0.67
Glutamine (Q)	0.5661	0.163	3.483	0.0
Glutamic acid (E)	0.5075	0.184	2.754	0.006
Glycine (G)	-0.3092	0.202	-1.533	0.125
Histidine (H)	0.3526	0.22	1.604	0.109
Isoleucine (I)	0.0765	0.185	0.415	0.679
Leucine (L)	0.1995	0.16	1.246	0.213
Lysine (K)	0.4769	0.169	2.815	0.005
Methionine (M)	0.3696	0.232	1.596	0.11
Phenylalanine (F)	0.4203	0.189	2.23	0.026
Proline (P)	0.3124	0.201	1.556	0.12
Serine (S)	0.3922	0.173	2.263	0.024
Threonine (T)	0.0548	0.197	0.278	0.781
Tryptophan (W)	0.4988	0.276	1.809	0.07
Tyrosine (Y)	0.2849	0.191	1.488	0.137
Vkabat	0.0783	0.018	4.293	0.0

Table B.91: Fields: Single-Assigned: isSwitch - E6 + isUnstruct + Vkabat

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13793
Df Model:	3
Date:	Thu Apr 04 16:28:34 PDT 2019
Pseudo R-squ.:	0.005778
Log-Likelihood:	-4187.3
LL-Null:	-4211.6
LLR p-value:	1.533E-10

Table B.92: Descriptors: Single-Assigned: isSwitch - E6 + isUnstruct + Vkabat

Name	**Beta**	**Std Err**	**Z-score**	**P-value**
Intercept	-2.653	0.075	-35.594	0.0
E6	0.2572	0.045	5.676	0.0
isUnstruct	-0.0621	0.122	-0.509	0.611
Vkabat	0.0754	0.018	4.176	0.0

Table B.93: Fields: Single-Assigned: isSwitch - E6 + Residue Type + Vkabat

Field	**Value**
Accuracy:	92.8130671506352
Df Residuals:	13775
Df Model:	21
Date:	Thu Apr 04 16:28:34 PDT 2019
Pseudo R-squ.:	0.01086
Log-Likelihood:	-4165.9
LL-Null:	-4211.6
LLR p-value:	9.028E-11

Table B.94: Descriptors: Single-Assigned: isSwitch - E6 + Residue Type + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.8948	0.144	-20.099	0.0
Alanine (A)	0.1297	0.172	0.754	0.451
Arginine (R)	0.2939	0.18	1.636	0.102
Asparagine (N)	0.3101	0.19	1.636	0.102
Aspartic acid (D)	0.3903	0.175	2.234	0.026
Cysteine (C)	0.0914	0.317	0.288	0.773
Glutamine (Q)	0.4726	0.164	2.884	0.004
Glutamic acid (E)	0.3893	0.186	2.092	0.036
Glycine (G)	-0.3731	0.202	-1.844	0.065
Histidine (H)	0.268	0.221	1.214	0.225
Isoleucine (I)	0.0884	0.185	0.479	0.632
Leucine (L)	0.2113	0.16	1.319	0.187
Lysine (K)	0.3908	0.171	2.292	0.022
Methionine (M)	0.3834	0.232	1.654	0.098
Phenylalanine (F)	0.4262	0.189	2.259	0.024
Proline (P)	0.2304	0.202	1.142	0.253
Serine (S)	0.2862	0.175	1.637	0.102
Threonine (T)	-0.0332	0.198	-0.168	0.867
Tryptophan (W)	0.5265	0.276	1.908	0.056
Tyrosine (Y)	0.295	0.192	1.54	0.124
E6	0.2389	0.048	5.023	0.0
Vkabat	0.0762	0.018	4.178	0.0

Table B.95: Fields: Single-Assigned: isSwitch - E6 + Residue Type + isUnstruct

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13775
Df Model:	21
Date:	Thu Apr 04 16:28:35 PDT 2019
Pseudo R-squ.:	0.009045
Log-Likelihood:	-4173.5
LL-Null:	-4211.6
LLR p-value:	3.465E-8

Table B.96: Descriptors: Single-Assigned: isSwitch - E6 + Residue Type + isUnstruct

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.6154	0.131	-19.939	0.0
Alanine (A)	0.1	0.172	0.582	0.561
Arginine (R)	0.3019	0.18	1.679	0.093
Asparagine (N)	0.2778	0.189	1.468	0.142
Aspartic acid (D)	0.359	0.175	2.056	0.04
Cysteine (C)	0.0738	0.317	0.233	0.816
Glutamine (Q)	0.4575	0.164	2.788	0.005
Glutamic acid (E)	0.3732	0.186	2.003	0.045
Glycine (G)	-0.4231	0.202	-2.096	0.036
Histidine (H)	0.261	0.221	1.183	0.237
Isoleucine (I)	0.0888	0.185	0.481	0.63
Leucine (L)	0.1893	0.16	1.183	0.237
Lysine (K)	0.3746	0.171	2.194	0.028
Methionine (M)	0.3918	0.233	1.685	0.092
Phenylalanine (F)	0.412	0.189	2.184	0.029
Proline (P)	0.1777	0.202	0.882	0.378
Serine (S)	0.2876	0.176	1.637	0.102
Threonine (T)	-0.0264	0.198	-0.134	0.894
Tryptophan (W)	0.521	0.276	1.888	0.059
Tyrosine (Y)	0.2748	0.192	1.435	0.151
E6	0.2473	0.048	5.194	0.0
isUnstruct	-0.1678	0.126	-1.333	0.183

Table B.97: Fields: Single-Assigned: isSwitch - E20 + isUnstruct + Vkabat

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13793
Df Model:	3
Date:	Thu Apr 04 16:28:35 PDT 2019
Pseudo R-squ.:	0.006775
Log-Likelihood:	-4183.1
LL-Null:	-4211.6
LLR p-value:	2.487E-12

Table B.98: Descriptors: Single-Assigned: isSwitch - E20 + isUnstruct + Vkabat

Name	**Beta**	**Std Err**	**Z-score**	**P-value**
Intercept	-2.6978	0.076	-35.426	0.0
E20	0.2071	0.032	6.381	0.0
isUnstruct	-0.0585	0.122	-0.48	0.631
Vkabat	0.0736	0.018	4.069	0.0

Table B.99: Fields: Single-Assigned: isSwitch - E20 + Residue Type + Vkabat

Field	**Value**
Accuracy:	92.8130671506352
Df Residuals:	13775
Df Model:	21
Date:	Thu Apr 04 16:28:35 PDT 2019
Pseudo R-squ.:	0.0122
Log-Likelihood:	-4160.3
LL-Null:	-4211.6
LLR p-value:	9.325E-13

Table B.100: Descriptors: Single-Assigned: isSwitch - E20 + Residue Type + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-3.0156	0.147	-20.521	0.0
Alanine (A)	0.2107	0.171	1.231	0.218
Arginine (R)	0.3739	0.179	2.092	0.036
Asparagine (N)	0.3834	0.189	2.031	0.042
Aspartic acid (D)	0.465	0.174	2.673	0.008
Cysteine (C)	0.1492	0.317	0.47	0.638
Glutamine (Q)	0.5535	0.163	3.401	0.001
Glutamic acid (E)	0.4773	0.185	2.585	0.01
Glycine (G)	-0.2544	0.202	-1.259	0.208
Histidine (H)	0.3487	0.22	1.584	0.113
Isoleucine (I)	0.0887	0.185	0.48	0.631
Leucine (L)	0.2635	0.161	1.64	0.101
Lysine (K)	0.4734	0.17	2.79	0.005
Methionine (M)	0.3996	0.232	1.723	0.085
Phenylalanine (F)	0.4947	0.189	2.616	0.009
Proline (P)	0.343	0.201	1.706	0.088
Serine (S)	0.3561	0.174	2.051	0.04
Threonine (T)	0.0176	0.197	0.089	0.929
Tryptophan (W)	0.622	0.277	2.246	0.025
Tyrosine (Y)	0.3624	0.192	1.887	0.059
E20	0.2003	0.033	6.07	0.0
Vkabat	0.0764	0.018	4.187	0.0

Table B.101: Fields: Single-Assigned: isSwitch - E20 + Residue Type + isUnstruct

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13775
Df Model:	21
Date:	Thu Apr 04 16:28:35 PDT 2019
Pseudo R-squ.:	0.0104
Log-Likelihood:	-4167.8
LL-Null:	-4211.6
LLR p-value:	4.127E-10

Table B.102: Descriptors: Single-Assigned: isSwitch - E20 + Residue Type + isUnstruct

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.7379	0.134	-20.366	0.0
Alanine (A)	0.1864	0.171	1.09	0.276
Arginine (R)	0.3865	0.179	2.16	0.031
Asparagine (N)	0.3562	0.189	1.889	0.059
Aspartic acid (D)	0.438	0.174	2.52	0.012
Cysteine (C)	0.1338	0.317	0.422	0.673
Glutamine (Q)	0.5436	0.163	3.332	0.001
Glutamic acid (E)	0.4672	0.185	2.525	0.012
Glycine (G)	-0.2993	0.202	-1.484	0.138
Histidine (H)	0.3457	0.22	1.571	0.116
Isoleucine (I)	0.0904	0.185	0.489	0.625
Leucine (L)	0.2439	0.161	1.52	0.129
Lysine (K)	0.4623	0.17	2.72	0.007
Methionine (M)	0.4096	0.233	1.76	0.078
Phenylalanine (F)	0.4828	0.189	2.553	0.011
Proline (P)	0.2966	0.201	1.475	0.14
Serine (S)	0.3628	0.175	2.078	0.038
Threonine (T)	0.0288	0.197	0.146	0.884
Tryptophan (W)	0.619	0.277	2.237	0.025
Tyrosine (Y)	0.3444	0.192	1.794	0.073
E20	0.2059	0.033	6.223	0.0
isUnstruct	-0.1774	0.126	-1.407	0.16

Table B.103: Fields: Single-Assigned: isSwitch - Residue Type + isUnstruct + Vkabat

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13775
Df Model:	21
Date:	Thu Apr 04 16:28:35 PDT 2019
Pseudo R-squ.:	0.007996
Log-Likelihood:	-4178.0
LL-Null:	-4211.6
LLR p-value:	9.282E-7

Table B.104: Descriptors: Single-Assigned: isSwitch - Residue Type + isUnstruct + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.8091	0.145	-19.334	0.0
Alanine (A)	0.2258	0.171	1.32	0.187
Arginine (R)	0.3899	0.179	2.181	0.029
Asparagine (N)	0.4032	0.189	2.138	0.032
Aspartic acid (D)	0.4796	0.174	2.758	0.006
Cysteine (C)	0.1304	0.317	0.412	0.681
Glutamine (Q)	0.5758	0.163	3.53	0.0
Glutamic acid (E)	0.518	0.185	2.802	0.005
Glycine (G)	-0.308	0.202	-1.527	0.127
Histidine (H)	0.3545	0.22	1.613	0.107
Isoleucine (I)	0.0757	0.185	0.41	0.682
Leucine (L)	0.2	0.16	1.249	0.212
Lysine (K)	0.4865	0.17	2.862	0.004
Methionine (M)	0.3851	0.233	1.656	0.098
Phenylalanine (F)	0.4154	0.189	2.202	0.028
Proline (P)	0.3249	0.202	1.612	0.107
Serine (S)	0.4057	0.174	2.327	0.02
Threonine (T)	0.0609	0.197	0.309	0.757
Tryptophan (W)	0.4919	0.276	1.783	0.075
Tyrosine (Y)	0.2796	0.192	1.46	0.144
isUnstruct	-0.0874	0.125	-0.697	0.486
Vkabat	0.0773	0.018	4.222	0.0

Table B.105: Fields: Single-Assigned: isSwitch - E6 + Residue Type + isUnstruct + Vkabat

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13774
Df Model:	22
Date:	Thu Apr 04 16:28:36 PDT 2019
Pseudo R-squ.:	0.01098
Log-Likelihood:	-4165.4
LL-Null:	-4211.6
LLR p-value:	1.293E-10

Table B.106: Descriptors: Single-Assigned: isSwitch - E6 + Residue Type + isUnstruct + Vkabat

Name	**Beta**	**Std Err**	**Z-score**	**P-value**
Intercept	-2.8694	0.146	-19.638	0.0
Alanine (A)	0.1357	0.172	0.788	0.431
Arginine (R)	0.3037	0.18	1.688	0.091
Asparagine (N)	0.3156	0.19	1.664	0.096
Aspartic acid (D)	0.3976	0.175	2.273	0.023
Cysteine (C)	0.0846	0.317	0.267	0.79
Glutamine (Q)	0.4852	0.164	2.952	0.003
Glutamic acid (E)	0.4023	0.187	2.156	0.031
Glycine (G)	-0.3719	0.202	-1.838	0.066
Histidine (H)	0.2696	0.221	1.221	0.222
Isoleucine (I)	0.0874	0.185	0.473	0.636
Leucine (L)	0.2122	0.16	1.324	0.186
Lysine (K)	0.4033	0.171	2.359	0.018
Methionine (M)	0.4051	0.233	1.741	0.082
Phenylalanine (F)	0.4192	0.189	2.221	0.026
Proline (P)	0.2476	0.202	1.223	0.221
Serine (S)	0.3048	0.176	1.734	0.083
Threonine (T)	-0.0256	0.198	-0.13	0.897
Tryptophan (W)	0.5166	0.276	1.87	0.061
Tyrosine (Y)	0.2875	0.192	1.5	0.134
E6	0.2419	0.048	5.078	0.0
isUnstruct	-0.1265	0.126	-1.003	0.316
Vkabat	0.0747	0.018	4.079	0.0

Table B.107: Fields: Single-Assigned: isSwitch - E20 + Residue Type + isUnstruct + Vkabat

Field	**Value**
Accuracy:	92.8130671506352
Df Residuals:	13774
Df Model:	22
Date:	Thu Apr 04 16:28:36 PDT 2019
Pseudo R-squ.:	0.01234
Log-Likelihood:	-4159.7
LL-Null:	-4211.6
LLR p-value:	1.306E-12

Table B.108: Descriptors: Single-Assigned: isSwitch - E20 + Residue Type + isUnstruct + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.9897	0.149	-20.094	0.0
Alanine (A)	0.2185	0.171	1.275	0.202
Arginine (R)	0.3858	0.179	2.154	0.031
Asparagine (N)	0.3906	0.189	2.068	0.039
Aspartic acid (D)	0.4741	0.174	2.723	0.006
Cysteine (C)	0.1427	0.317	0.45	0.653
Glutamine (Q)	0.5683	0.163	3.479	0.001
Glutamic acid (E)	0.4926	0.185	2.66	0.008
Glycine (G)	-0.2514	0.202	-1.244	0.214
Histidine (H)	0.3518	0.22	1.598	0.11
Isoleucine (I)	0.0878	0.185	0.475	0.635
Leucine (L)	0.2651	0.161	1.65	0.099
Lysine (K)	0.4881	0.17	2.868	0.004
Methionine (M)	0.4227	0.233	1.815	0.07
Phenylalanine (F)	0.4879	0.189	2.578	0.01
Proline (P)	0.3631	0.202	1.799	0.072
Serine (S)	0.3774	0.175	2.16	0.031
Threonine (T)	0.0267	0.197	0.136	0.892
Tryptophan (W)	0.6123	0.277	2.21	0.027
Tyrosine (Y)	0.3552	0.192	1.849	0.065
E20	0.2027	0.033	6.129	0.0
isUnstruct	-0.1366	0.126	-1.081	0.279
Vkabat	0.0748	0.018	4.083	0.0

Table B.109: Fields: Single-Unassigned: isSwitch - Residue Type

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13777
Df Model:	19
Date:	Thu Apr 04 16:28:44 PDT 2019
Pseudo R-squ.:	0.01934
Log-Likelihood:	-2228.9
LL-Null:	-2272.8
LLR p-value:	7.686E-11

Table B.110: Descriptors: Single-Unassigned: isSwitch - Residue Type

Name	Beta	Std Err	Z-score	P-value
Intercept	-4.2363	0.279	-15.165	0.0
Alanine (A)	1.2816	0.314	4.08	0.0
Arginine (R)	0.7269	0.356	2.039	0.041
Asparagine (N)	1.2989	0.336	3.862	0.0
Aspartic acid (D)	1.366	0.321	4.252	0.0
Cysteine (C)	0.9782	0.501	1.952	0.051
Glutamine (Q)	1.1071	0.321	3.451	0.001
Glutamic acid (E)	1.1558	0.344	3.361	0.001
Glycine (G)	1.0389	0.33	3.152	0.002
Histidine (H)	0.6867	0.425	1.615	0.106
Isoleucine (I)	0.51	0.363	1.404	0.16
Leucine (L)	0.7035	0.321	2.191	0.028
Lysine (K)	1.4819	0.314	4.722	0.0
Methionine (M)	1.5213	0.366	4.154	0.0
Phenylalanine (F)	0.2182	0.424	0.514	0.607
Proline (P)	1.2699	0.344	3.689	0.0
Serine (S)	1.5321	0.314	4.88	0.0
Threonine (T)	1.203	0.336	3.579	0.0
Tryptophan (W)	0.5228	0.578	0.904	0.366
Tyrosine (Y)	0.1605	0.424	0.379	0.705

Table B.111: Fields: Single-Unassigned: isSwitch - E6

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13795
Df Model:	1
Date:	Thu Apr 04 16:28:44 PDT 2019
Pseudo R-squ.:	0.01429
Log-Likelihood:	-2240.4
LL-Null:	-2272.8
LLR p-value:	7.680E-16

Table B.112: Descriptors: Single-Unassigned: isSwitch - E6

Name	Beta	Std Err	Z-score	P-value
Intercept	-3.5214	0.063	-55.917	0.0
E6	0.5247	0.063	8.311	0.0

Table B.113: Fields: Single-Unassigned: isSwitch - E20

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13795
Df Model:	1
Date:	Thu Apr 04 16:28:45 PDT 2019
Pseudo R-squ.:	0.01612
Log-Likelihood:	-2236.2
LL-Null:	-2272.8
LLR p-value:	1.121E-17

Table B.114: Descriptors: Single-Unassigned: isSwitch - E20

Name	Beta	Std Err	Z-score	P-value
Intercept	-3.6073	0.069	-52.208	0.0
E20	0.4029	0.046	8.779	0.0

Table B.115: Fields: Single-Unassigned: isSwitch - isUnstruct

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13795
Df Model:	1
Date:	Thu Apr 04 16:28:45 PDT 2019
Pseudo R-squ.:	0.1194
Log-Likelihood:	-2001.5
LL-Null:	-2272.8
LLR p-value:	4.898E-120

Table B.116: Descriptors: Single-Unassigned: isSwitch - isUnstruct

Name	Beta	Std Err	Z-score	P-value
Intercept	-4.316	0.079	-54.608	0.0
isUnstruct	3.2266	0.134	24.046	0.0

Table B.117: Fields: Single-Unassigned: isSwitch - Vkabat

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13795
Df Model:	1
Date:	Thu Apr 04 16:28:45 PDT 2019
Pseudo R-squ.:	0.005996
Log-Likelihood:	-2259.2
LL-Null:	-2272.8
LLR p-value:	1.782E-7

Table B.118: Descriptors: Single-Unassigned: isSwitch - Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.7771	0.091	-30.461	0.0
Vkabat	-0.1543	0.031	-5.047	0.0

Table B.119: Fields: Single-Unassigned: isSwitch - E6 + Residue Type

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13776
Df Model:	20
Date:	Thu Apr 04 16:28:45 PDT 2019
Pseudo R-squ.:	0.02814
Log-Likelihood:	-2208.9
LL-Null:	-2272.8
LLR p-value:	9.604E-18

Table B.120: Descriptors: Single-Unassigned: isSwitch - E6 + Residue Type

Name	Beta	Std Err	Z-score	P-value
Intercept	-4.3804	0.281	-15.606	0.0
Alanine (A)	1.1104	0.316	3.518	0.0
Arginine (R)	0.5506	0.358	1.538	0.124
Asparagine (N)	1.1316	0.338	3.349	0.001
Aspartic acid (D)	1.2045	0.323	3.733	0.0
Cysteine (C)	0.8929	0.502	1.779	0.075
Glutamine (Q)	0.9288	0.322	2.881	0.004
Glutamic acid (E)	0.933	0.346	2.695	0.007
Glycine (G)	0.9154	0.331	2.769	0.006
Histidine (H)	0.521	0.427	1.221	0.222
Isoleucine (I)	0.5304	0.363	1.459	0.144
Leucine (L)	0.7272	0.321	2.263	0.024
Lysine (K)	1.3174	0.315	4.178	0.0
Methionine (M)	1.5492	0.367	4.226	0.0
Phenylalanine (F)	0.228	0.424	0.537	0.591
Proline (P)	1.1152	0.346	3.227	0.001
Serine (S)	1.3325	0.316	4.219	0.0
Threonine (T)	1.0334	0.338	3.061	0.002
Tryptophan (W)	0.5709	0.578	0.987	0.324
Tyrosine (Y)	0.1756	0.424	0.414	0.679
E6	0.4315	0.067	6.445	0.0

Table B.121: Fields: Single-Unassigned: isSwitch - E6 + isUnstruct

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13794
Df Model:	2
Date:	Thu Apr 04 16:28:45 PDT 2019
Pseudo R-squ.:	0.1267
Log-Likelihood:	-1984.9
LL-Null:	-2272.8
LLR p-value:	9.104E-126

Table B.122: Descriptors: Single-Unassigned: isSwitch - E6 + isUnstruct

Name	Beta	Std Err	Z-score	P-value
Intercept	-4.5352	0.091	-50.072	0.0
E6	0.3928	0.067	5.87	0.0
isUnstruct	3.1644	0.136	23.331	0.0

Table B.123: Fields: Single-Unassigned: isSwitch - E6 + Vkabat

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13794
Df Model:	2
Date:	Thu Apr 04 16:28:45 PDT 2019
Pseudo R-squ.:	0.02023
Log-Likelihood:	-2226.8
LL-Null:	-2272.8
LLR p-value:	1.068E-20

Table B.124: Descriptors: Single-Unassigned: isSwitch - E6 + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-3.0962	0.102	-30.453	0.0
E6	0.5247	0.063	8.293	0.0
Vkabat	-0.1535	0.031	-5.025	0.0

Table B.125: Fields: Single-Unassigned: isSwitch - E20 + Residue Type

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13776
Df Model:	20
Date:	Thu Apr 04 16:28:45 PDT 2019
Pseudo R-squ.:	0.03226
Log-Likelihood:	-2199.5
LL-Null:	-2272.8
LLR p-value:	2.765E-21

Table B.126: Descriptors: Single-Unassigned: isSwitch - E20 + Residue Type

Name	Beta	Std Err	Z-score	P-value
Intercept	-4.6138	0.285	-16.205	0.0
Alanine (A)	1.2625	0.314	4.014	0.0
Arginine (R)	0.696	0.357	1.95	0.051
Asparagine (N)	1.2663	0.337	3.758	0.0
Aspartic acid (D)	1.3433	0.322	4.176	0.0
Cysteine (C)	0.9952	0.502	1.982	0.047
Glutamine (Q)	1.0788	0.321	3.359	0.001
Glutamic acid (E)	1.0936	0.345	3.174	0.002
Glycine (G)	1.1391	0.33	3.449	0.001
Histidine (H)	0.6694	0.426	1.571	0.116
Isoleucine (I)	0.5343	0.364	1.47	0.142
Leucine (L)	0.825	0.322	2.563	0.01
Lysine (K)	1.4706	0.314	4.68	0.0
Methionine (M)	1.578	0.367	4.3	0.0
Phenylalanine (F)	0.3554	0.425	0.837	0.403
Proline (P)	1.3254	0.345	3.844	0.0
Serine (S)	1.4613	0.314	4.647	0.0
Threonine (T)	1.1262	0.337	3.344	0.001
Tryptophan (W)	0.7484	0.579	1.291	0.197
Tyrosine (Y)	0.3013	0.425	0.71	0.478
E20	0.3665	0.047	7.814	0.0

Table B.127: Fields: Single-Unassigned: isSwitch - E20 + isUnstruct

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13794
Df Model:	2
Date:	Thu Apr 04 16:28:45 PDT 2019
Pseudo R-squ.:	0.1296
Log-Likelihood:	-1978.2
LL-Null:	-2272.8
LLR p-value:	1.111E-128

Table B.128: Descriptors: Single-Unassigned: isSwitch - E20 + isUnstruct

Name	Beta	Std Err	Z-score	P-value
Intercept	-4.6396	0.096	-48.252	0.0
E20	0.3346	0.048	6.943	0.0
isUnstruct	3.1817	0.136	23.426	0.0

Table B.129: Fields: Single-Unassigned: isSwitch - E20 + Vkabat

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13794
Df Model:	2
Date:	Thu Apr 04 16:28:45 PDT 2019
Pseudo R-squ.:	0.0225
Log-Likelihood:	-2221.7
LL-Null:	-2272.8
LLR p-value:	6.210E-23

Table B.130: Descriptors: Single-Unassigned: isSwitch - E20 + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-3.173	0.105	-30.298	0.0
E20	0.4096	0.046	8.879	0.0
Vkabat	-0.1593	0.031	-5.199	0.0

Table B.131: Fields: Single-Unassigned: isSwitch - isUnstruct + Vkabat

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13794
Df Model:	2
Date:	Thu Apr 04 16:28:46 PDT 2019
Pseudo R-squ.:	0.1214
Log-Likelihood:	-1996.8
LL-Null:	-2272.8
LLR p-value:	1.326E-120

Table B.132: Descriptors: Single-Unassigned: isSwitch - isUnstruct + Vkabat

Name	**Beta**	**Std Err**	**Z-score**	**P-value**
Intercept	-4.0405	0.118	-34.135	0.0
isUnstruct	3.1862	0.135	23.625	0.0
Vkabat	-0.0944	0.031	-3.004	0.003

Table B.133: Fields: Single-Unassigned: isSwitch - isUnstruct + Residue Type

Field	**Value**
Accuracy:	91.36116152450091
Df Residuals:	13776
Df Model:	20
Date:	Thu Apr 04 16:28:46 PDT 2019
Pseudo R-squ.:	0.1263
Log-Likelihood:	-1985.7
LL-Null:	-2272.8
LLR p-value:	7.452E-109

Table B.134: Descriptors: Single-Unassigned: isSwitch - isUnstruct + Residue Type

Name	Beta	Std Err	Z-score	P-value
Intercept	-5.0784	0.288	-17.642	0.0
Alanine (A)	1.0538	0.319	3.3	0.001
Arginine (R)	0.3801	0.362	1.049	0.294
Asparagine (N)	1.0274	0.344	2.99	0.003
Aspartic acid (D)	1.0962	0.327	3.352	0.001
Cysteine (C)	1.2425	0.51	2.437	0.015
Glutamine (Q)	0.6436	0.326	1.972	0.049
Glutamic acid (E)	0.6442	0.351	1.836	0.066
Glycine (G)	0.969	0.335	2.893	0.004
Histidine (H)	0.6453	0.431	1.496	0.135
Isoleucine (I)	0.5757	0.368	1.563	0.118
Leucine (L)	0.6859	0.325	2.108	0.035
Lysine (K)	1.0117	0.32	3.16	0.002
Methionine (M)	0.6898	0.378	1.822	0.068
Phenylalanine (F)	0.5319	0.429	1.24	0.215
Proline (P)	0.6516	0.352	1.854	0.064
Serine (S)	0.9039	0.321	2.819	0.005
Threonine (T)	0.931	0.342	2.72	0.007
Tryptophan (W)	0.9499	0.586	1.62	0.105
Tyrosine (Y)	0.4869	0.429	1.136	0.256
isUnstruct	3.1815	0.141	22.533	0.0

Table B.135: Fields: Single-Unassigned: isSwitch - Vkabat + Residue Type

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13776
Df Model:	20
Date:	Thu Apr 04 16:28:46 PDT 2019
Pseudo R-squ.:	0.02386
Log-Likelihood:	-2218.6
LL-Null:	-2272.8
LLR p-value:	3.780E-14

Table B.136: Descriptors: Single-Unassigned: isSwitch - Vkabat + Residue Type

Name	Beta	Std Err	Z-score	P-value
Intercept	-3.8203	0.293	-13.022	0.0
Alanine (A)	1.2217	0.315	3.885	0.0
Arginine (R)	0.7239	0.357	2.03	0.042
Asparagine (N)	1.2429	0.337	3.692	0.0
Aspartic acid (D)	1.3129	0.322	4.083	0.0
Cysteine (C)	0.9704	0.501	1.935	0.053
Glutamine (Q)	1.0573	0.321	3.293	0.001
Glutamic acid (E)	1.1051	0.344	3.21	0.001
Glycine (G)	0.9615	0.33	2.912	0.004
Histidine (H)	0.6789	0.426	1.595	0.111
Isoleucine (I)	0.5165	0.363	1.421	0.155
Leucine (L)	0.6631	0.321	2.063	0.039
Lysine (K)	1.4355	0.314	4.57	0.0
Methionine (M)	1.491	0.367	4.068	0.0
Phenylalanine (F)	0.2158	0.424	0.509	0.611
Proline (P)	1.1534	0.345	3.342	0.001
Serine (S)	1.5066	0.314	4.796	0.0
Threonine (T)	1.2059	0.336	3.586	0.0
Tryptophan (W)	0.5372	0.578	0.929	0.353
Tyrosine (Y)	0.1505	0.424	0.355	0.723
Vkabat	-0.1366	0.031	-4.399	0.0

Table B.137: Fields: Single-Unassigned: isSwitch - E6 + isUnstruct + Vkabat

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13793
Df Model:	3
Date:	Thu Apr 04 16:28:46 PDT 2019
Pseudo R-squ.:	0.1287
Log-Likelihood:	-1980.3
LL-Null:	-2272.8
LLR p-value:	1.785E-126

Table B.138: Descriptors: Single-Unassigned: isSwitch - E6 + isUnstruct + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-4.2614	0.127	-33.678	0.0
E6	0.3921	0.067	5.853	0.0
isUnstruct	3.1235	0.136	22.906	0.0
Vkabat	-0.0935	0.031	-2.975	0.003

Table B.139: Fields: Single-Unassigned: isSwitch - E6 + Residue Type + Vkabat

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13775
Df Model:	21
Date:	Thu Apr 04 16:28:46 PDT 2019
Pseudo R-squ.:	0.03278
Log-Likelihood:	-2198.3
LL-Null:	-2272.8
LLR p-value:	2.733E-21

Table B.140: Descriptors: Single-Unassigned: isSwitch - E6 + Residue Type + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-3.9541	0.295	-13.412	0.0
Alanine (A)	1.0423	0.316	3.296	0.001
Arginine (R)	0.5378	0.358	1.5	0.133
Asparagine (N)	1.0689	0.338	3.16	0.002
Aspartic acid (D)	1.1353	0.323	3.512	0.0
Cysteine (C)	0.8754	0.502	1.743	0.081
Glutamine (Q)	0.8749	0.323	2.71	0.007
Glutamic acid (E)	0.8762	0.347	2.528	0.011
Glycine (G)	0.8244	0.331	2.488	0.013
Histidine (H)	0.5065	0.427	1.186	0.236
Isoleucine (I)	0.5319	0.364	1.463	0.143
Leucine (L)	0.6829	0.322	2.124	0.034
Lysine (K)	1.2609	0.316	3.993	0.0
Methionine (M)	1.5154	0.367	4.131	0.0
Phenylalanine (F)	0.2193	0.424	0.517	0.605
Proline (P)	0.9892	0.347	2.853	0.004
Serine (S)	1.2951	0.316	4.095	0.0
Threonine (T)	1.0239	0.338	3.03	0.002
Tryptophan (W)	0.58	0.579	1.002	0.316
Tyrosine (Y)	0.1576	0.424	0.372	0.71
E6	0.4359	0.067	6.491	0.0
Vkabat	-0.1382	0.031	-4.458	0.0

Table B.141: Fields: Single-Unassigned: isSwitch - E6 + Residue Type + isUnstruct

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13775
Df Model:	21
Date:	Thu Apr 04 16:28:46 PDT 2019
Pseudo R-squ.:	0.1324
Log-Likelihood:	-1972.0
LL-Null:	-2272.8
LLR p-value:	6.888E-114

Table B.142: Descriptors: Single-Unassigned: isSwitch - E6 + Residue Type + isUnstruct

Name	Beta	Std Err	Z-score	P-value
Intercept	-5.2101	0.29	-17.965	0.0
Alanine (A)	0.9056	0.321	2.818	0.005
Arginine (R)	0.2454	0.364	0.674	0.5
Asparagine (N)	0.8859	0.346	2.563	0.01
Aspartic acid (D)	0.9819	0.328	2.992	0.003
Cysteine (C)	1.1588	0.513	2.26	0.024
Glutamine (Q)	0.524	0.328	1.6	0.11
Glutamic acid (E)	0.5013	0.352	1.423	0.155
Glycine (G)	0.8495	0.337	2.523	0.012
Histidine (H)	0.497	0.434	1.145	0.252
Isoleucine (I)	0.6008	0.369	1.629	0.103
Leucine (L)	0.7126	0.326	2.186	0.029
Lysine (K)	0.9021	0.321	2.809	0.005
Methionine (M)	0.7736	0.378	2.045	0.041
Phenylalanine (F)	0.5415	0.429	1.261	0.207
Proline (P)	0.5271	0.353	1.493	0.135
Serine (S)	0.7295	0.323	2.258	0.024
Threonine (T)	0.8072	0.344	2.349	0.019
Tryptophan (W)	1.0152	0.586	1.732	0.083
Tyrosine (Y)	0.5042	0.429	1.174	0.24
E6	0.3748	0.071	5.315	0.0
isUnstruct	3.1528	0.142	22.242	0.0

Table B.143: Fields: Single-Unassigned: isSwitch - E20 + isUnstruct + Vkabat

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13793
Df Model:	3
Date:	Thu Apr 04 16:28:47 PDT 2019
Pseudo R-squ.:	0.132
Log-Likelihood:	-1972.9
LL-Null:	-2272.8
LLR p-value:	1.098E-129

Table B.144: Descriptors: Single-Unassigned: isSwitch - E20 + isUnstruct + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-4.3519	0.129	-33.663	0.0
E20	0.34	0.048	7.033	0.0
isUnstruct	3.1384	0.137	22.987	0.0
Vkabat	-0.1004	0.031	-3.189	0.001

Table B.145: Fields: Single-Unassigned: isSwitch - E20 + Residue Type + Vkabat

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13775
Df Model:	21
Date:	Thu Apr 04 16:28:47 PDT 2019
Pseudo R-squ.:	0.03697
Log-Likelihood:	-2188.8
LL-Null:	-2272.8
LLR p-value:	6.060E-25

Table B.146: Descriptors: Single-Unassigned: isSwitch - E20 + Residue Type + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-4.1899	0.298	-14.046	0.0
Alanine (A)	1.2008	0.315	3.813	0.0
Arginine (R)	0.6862	0.357	1.921	0.055
Asparagine (N)	1.2094	0.337	3.586	0.0
Aspartic acid (D)	1.2769	0.322	3.964	0.0
Cysteine (C)	0.9811	0.502	1.952	0.051
Glutamine (Q)	1.0293	0.321	3.202	0.001
Glutamic acid (E)	1.0427	0.345	3.023	0.002
Glycine (G)	1.0526	0.331	3.182	0.001
Histidine (H)	0.6576	0.426	1.543	0.123
Isoleucine (I)	0.5396	0.364	1.484	0.138
Leucine (L)	0.7844	0.322	2.436	0.015
Lysine (K)	1.4186	0.315	4.51	0.0
Methionine (M)	1.5451	0.367	4.207	0.0
Phenylalanine (F)	0.351	0.425	0.826	0.409
Proline (P)	1.2042	0.346	3.483	0.0
Serine (S)	1.4274	0.315	4.535	0.0
Threonine (T)	1.1218	0.337	3.328	0.001
Tryptophan (W)	0.7625	0.58	1.315	0.188
Tyrosine (Y)	0.2875	0.425	0.677	0.499
E20	0.3711	0.047	7.874	0.0
Vkabat	-0.1396	0.031	-4.496	0.0

Table B.147: Fields: Single-Unassigned: isSwitch - E20 + Residue Type + isUnstruct

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13775
Df Model:	21
Date:	Thu Apr 04 16:28:47 PDT 2019
Pseudo R-squ.:	0.1361
Log-Likelihood:	-1963.5
LL-Null:	-2272.8
LLR p-value:	1.870E-117

Table B.148: Descriptors: Single-Unassigned: isSwitch - E20 + Residue Type + isUnstruct

Name	Beta	Std Err	Z-score	P-value
Intercept	-5.4225	0.294	-18.438	0.0
Alanine (A)	1.0252	0.32	3.202	0.001
Arginine (R)	0.3558	0.363	0.98	0.327
Asparagine (N)	0.9883	0.345	2.867	0.004
Aspartic acid (D)	1.087	0.328	3.318	0.001
Cysteine (C)	1.2458	0.513	2.428	0.015
Glutamine (Q)	0.6511	0.327	1.993	0.046
Glutamic acid (E)	0.6397	0.351	1.822	0.068
Glycine (G)	1.0345	0.336	3.078	0.002
Histidine (H)	0.6064	0.434	1.399	0.162
Isoleucine (I)	0.5889	0.369	1.597	0.11
Leucine (L)	0.7908	0.326	2.423	0.015
Lysine (K)	1.029	0.32	3.211	0.001
Methionine (M)	0.8365	0.378	2.214	0.027
Phenylalanine (F)	0.6538	0.43	1.521	0.128
Proline (P)	0.7054	0.352	2.002	0.045
Serine (S)	0.8278	0.322	2.573	0.01
Threonine (T)	0.8712	0.343	2.539	0.011
Tryptophan (W)	1.178	0.587	2.008	0.045
Tyrosine (Y)	0.6134	0.43	1.428	0.153
E20	0.3335	0.049	6.767	0.0
isUnstruct	3.1547	0.142	22.191	0.0

Table B.149: Fields: Single-Unassigned: isSwitch - Residue Type + isUnstruct + Vkabat

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13775
Df Model:	21
Date:	Thu Apr 04 16:28:47 PDT 2019
Pseudo R-squ.:	0.1278
Log-Likelihood:	-1982.3
LL-Null:	-2272.8
LLR p-value:	1.583E-109

Table B.150: Descriptors: Single-Unassigned: isSwitch - Residue Type + isUnstruct + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-4.8031	0.306	-15.706	0.0
Alanine (A)	1.007	0.32	3.15	0.002
Arginine (R)	0.3712	0.362	1.025	0.306
Asparagine (N)	0.9676	0.345	2.808	0.005
Aspartic acid (D)	1.0434	0.328	3.184	0.001
Cysteine (C)	1.2098	0.51	2.37	0.018
Glutamine (Q)	0.5993	0.327	1.834	0.067
Glutamic acid (E)	0.5933	0.351	1.688	0.091
Glycine (G)	0.892	0.336	2.653	0.008
Histidine (H)	0.6176	0.432	1.431	0.152
Isoleucine (I)	0.5819	0.368	1.581	0.114
Leucine (L)	0.6523	0.326	2.004	0.045
Lysine (K)	0.9746	0.32	3.042	0.002
Methionine (M)	0.6659	0.379	1.759	0.079
Phenylalanine (F)	0.5163	0.429	1.204	0.228
Proline (P)	0.5663	0.353	1.604	0.109
Serine (S)	0.8678	0.321	2.703	0.007
Threonine (T)	0.9182	0.342	2.682	0.007
Tryptophan (W)	0.9384	0.587	1.6	0.11
Tyrosine (Y)	0.4673	0.429	1.09	0.276
isUnstruct	3.1502	0.142	22.209	0.0
Vkabat	-0.0818	0.032	-2.55	0.011

Table B.151: Fields: Single-Unassigned: isSwitch - E6 + Residue Type + isUnstruct + Vkabat

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13774
Df Model:	22
Date:	Thu Apr 04 16:28:47 PDT 2019
Pseudo R-squ.:	0.134
Log-Likelihood:	-1968.3
LL-Null:	-2272.8
LLR p-value:	1.127E-114

Table B.152: Descriptors: Single-Unassigned: isSwitch - E6 + Residue Type + isUnstruct + Vkabat

Name	**Beta**	**Std Err**	**Z-score**	**P-value**
Intercept	-4.924	0.308	-15.996	0.0
Alanine (A)	0.8538	0.322	2.652	0.008
Arginine (R)	0.2312	0.364	0.635	0.525
Asparagine (N)	0.8224	0.347	2.373	0.018
Aspartic acid (D)	0.9215	0.329	2.801	0.005
Cysteine (C)	1.1214	0.513	2.185	0.029
Glutamine (Q)	0.4766	0.328	1.453	0.146
Glutamic acid (E)	0.4453	0.353	1.262	0.207
Glycine (G)	0.7646	0.338	2.26	0.024
Histidine (H)	0.4652	0.434	1.071	0.284
Isoleucine (I)	0.6051	0.369	1.642	0.101
Leucine (L)	0.6776	0.326	2.077	0.038
Lysine (K)	0.8601	0.322	2.675	0.007
Methionine (M)	0.7481	0.378	1.977	0.048
Phenylalanine (F)	0.5245	0.429	1.222	0.222
Proline (P)	0.4354	0.355	1.227	0.22
Serine (S)	0.6875	0.324	2.124	0.034
Threonine (T)	0.7889	0.344	2.295	0.022
Tryptophan (W)	1.0027	0.586	1.71	0.087
Tyrosine (Y)	0.4823	0.429	1.124	0.261
E6	0.3789	0.071	5.367	0.0
isUnstruct	3.1208	0.142	21.915	0.0
Vkabat	-0.085	0.032	-2.649	0.008

Table B.153: Fields: Single-Unassigned: isSwitch - E20 + Residue Type + isUnstruct + Vkabat

Field	**Value**
Accuracy:	91.36116152450091
Df Residuals:	13774
Df Model:	22
Date:	Thu Apr 04 16:28:48 PDT 2019
Pseudo R-squ.:	0.1378
Log-Likelihood:	-1959.7
LL-Null:	-2272.8
LLR p-value:	2.557E-118

Table B.154: Descriptors: Single-Unassigned: isSwitch - E20 + Residue Type + isUnstruct + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-5.1321	0.311	-16.493	0.0
Alanine (A)	0.9746	0.321	3.04	0.002
Arginine (R)	0.3417	0.363	0.941	0.347
Asparagine (N)	0.9258	0.346	2.679	0.007
Aspartic acid (D)	1.0255	0.328	3.124	0.002
Cysteine (C)	1.2085	0.514	2.353	0.019
Glutamine (Q)	0.604	0.327	1.847	0.065
Glutamic acid (E)	0.5839	0.352	1.66	0.097
Glycine (G)	0.9495	0.337	2.814	0.005
Histidine (H)	0.5741	0.434	1.323	0.186
Isoleucine (I)	0.5944	0.369	1.613	0.107
Leucine (L)	0.7561	0.327	2.315	0.021
Lysine (K)	0.9876	0.321	3.079	0.002
Methionine (M)	0.81	0.378	2.143	0.032
Phenylalanine (F)	0.6375	0.43	1.484	0.138
Proline (P)	0.6139	0.354	1.735	0.083
Serine (S)	0.786	0.322	2.44	0.015
Threonine (T)	0.8533	0.343	2.486	0.013
Tryptophan (W)	1.167	0.587	1.988	0.047
Tyrosine (Y)	0.5917	0.43	1.377	0.168
E20	0.3379	0.049	6.837	0.0
isUnstruct	3.1221	0.143	21.864	0.0
Vkabat	-0.0874	0.032	-2.719	0.007

Table B.155: Fields: Triplet-Both: isSwitch - Residue Type

Field	Value
Accuracy:	84.17422867513612
Df Residuals:	13777
Df Model:	19
Date:	Thu Apr 04 16:28:57 PDT 2019
Pseudo R-squ.:	0.007754
Log-Likelihood:	-5294.1
LL-Null:	-5335.5
LLR p-value:	6.227E-10

Table B.156: Descriptors: Triplet-Both: isSwitch - Residue Type

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.3695	0.118	-20.012	0.0
Alanine (A)	0.5033	0.15	3.364	0.001
Arginine (R)	0.4687	0.162	2.893	0.004
Asparagine (N)	0.6296	0.165	3.816	0.0
Aspartic acid (D)	0.7086	0.153	4.619	0.0
Cysteine (C)	0.3511	0.271	1.294	0.196
Glutamine (Q)	0.694	0.147	4.729	0.0
Glutamic acid (E)	0.6638	0.164	4.039	0.0
Glycine (G)	0.0567	0.168	0.338	0.735
Histidine (H)	0.43	0.199	2.165	0.03
Isoleucine (I)	0.175	0.167	1.051	0.293
Leucine (L)	0.3009	0.145	2.078	0.038
Lysine (K)	0.7615	0.149	5.099	0.0
Methionine (M)	0.7123	0.196	3.639	0.0
Phenylalanine (F)	0.395	0.175	2.261	0.024
Proline (P)	0.5331	0.173	3.083	0.002
Serine (S)	0.7323	0.151	4.843	0.0
Threonine (T)	0.3863	0.169	2.292	0.022
Tryptophan (W)	0.5283	0.254	2.082	0.037
Tyrosine (Y)	0.2635	0.177	1.49	0.136

Table B.157: Fields: Triplet-Both: isSwitch - E6

Field	Value
Accuracy:	84.17422867513612
Df Residuals:	13795
Df Model:	1
Date:	Thu Apr 04 16:28:57 PDT 2019
Pseudo R-squ.:	0.01297
Log-Likelihood:	-5266.3
LL-Null:	-5335.5
LLR p-value:	5.835E-32

Table B.158: Descriptors: Triplet-Both: isSwitch - E6

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.246	0.041	-55.421	0.0
E6	0.6282	0.053	11.965	0.0

Table B.159: Fields: Triplet-Both: isSwitch - E20

Field	Value
Accuracy:	84.17422867513612
Df Residuals:	13795
Df Model:	1
Date:	Thu Apr 04 16:28:57 PDT 2019
Pseudo R-squ.:	0.0134
Log-Likelihood:	-5264.0
LL-Null:	-5335.5
LLR p-value:	5.845E-33

Table B.160: Descriptors: Triplet-Both: isSwitch - E20

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.2988	0.044	-52.56	0.0
E20	0.4327	0.036	12.127	0.0

Table B.161: Fields: Triplet-Both: isSwitch - isUnstruct

Field	Value
Accuracy:	84.17422867513612
Df Residuals:	13795
Df Model:	1
Date:	Thu Apr 04 16:28:57 PDT 2019
Pseudo R-squ.:	0.0199
Log-Likelihood:	-5229.3
LL-Null:	-5335.5
LLR p-value:	4.223E-48

Table B.162: Descriptors: Triplet-Both: isSwitch - isUnstruct

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.2454	0.036	-61.88	0.0
isUnstruct	1.3471	0.089	15.126	0.0

Table B.163: Fields: Triplet-Both: isSwitch - Vkabat

Field	Value
Accuracy:	84.17422867513612
Df Residuals:	13795
Df Model:	1
Date:	Thu Apr 04 16:28:57 PDT 2019
Pseudo R-squ.:	4.759E-5
Log-Likelihood:	-5335.3
LL-Null:	-5335.5
LLR p-value:	0.4761

Table B.164: Descriptors: Triplet-Both: isSwitch - Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-1.9329	0.053	-36.218	0.0
Vkabat	0.0113	0.016	0.714	0.475

Table B.165: Fields: Triplet-Both: isSwitch - E6 + Residue Type

Field	Value
Accuracy:	84.17422867513612
Df Residuals:	13776
Df Model:	20
Date:	Thu Apr 04 16:28:57 PDT 2019
Pseudo R-squ.:	0.01889
Log-Likelihood:	-5234.7
LL-Null:	-5335.5
LLR p-value:	5.577E-32

Table B.166: Descriptors: Triplet-Both: isSwitch - E6 + Residue Type

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.6374	0.122	-21.685	0.0
Alanine (A)	0.4138	0.15	2.752	0.006
Arginine (R)	0.3659	0.163	2.246	0.025
Asparagine (N)	0.5395	0.166	3.252	0.001
Aspartic acid (D)	0.5897	0.154	3.818	0.0
Cysteine (C)	0.3009	0.273	1.104	0.27
Glutamine (Q)	0.5963	0.148	4.04	0.0
Glutamic acid (E)	0.5736	0.165	3.472	0.001
Glycine (G)	-0.024	0.168	-0.143	0.887
Histidine (H)	0.3545	0.199	1.777	0.076
Isoleucine (I)	0.1853	0.167	1.11	0.267
Leucine (L)	0.3165	0.145	2.179	0.029
Lysine (K)	0.6832	0.15	4.552	0.0
Methionine (M)	0.7173	0.196	3.651	0.0
Phenylalanine (F)	0.4009	0.175	2.288	0.022
Proline (P)	0.4237	0.174	2.435	0.015
Serine (S)	0.6237	0.152	4.1	0.0
Threonine (T)	0.3132	0.169	1.85	0.064
Tryptophan (W)	0.5726	0.255	2.249	0.025
Tyrosine (Y)	0.2897	0.177	1.634	0.102
E6	0.5923	0.054	11.051	0.0

Table B.167: Fields: Triplet-Both: isSwitch - E6 + isUnstruct

Field	Value
Accuracy:	84.17422867513612
Df Residuals:	13794
Df Model:	2
Date:	Thu Apr 04 16:28:58 PDT 2019
Pseudo R-squ.:	0.02851
Log-Likelihood:	-5183.4
LL-Null:	-5335.5
LLR p-value:	8.792E-67

Table B.168: Descriptors: Triplet-Both: isSwitch - E6 + isUnstruct

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.4989	0.046	-54.037	0.0
E6	0.5217	0.054	9.722	0.0
isUnstruct	1.2123	0.091	13.321	0.0

Table B.169: Fields: Triplet-Both: isSwitch - E6 + Vkabat

Field	Value
Accuracy:	84.17422867513612
Df Residuals:	13794
Df Model:	2
Date:	Thu Apr 04 16:28:58 PDT 2019
Pseudo R-squ.:	0.01306
Log-Likelihood:	-5265.8
LL-Null:	-5335.5
LLR p-value:	5.439E-31

Table B.170: Descriptors: Triplet-Both: isSwitch - E6 + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.2921	0.063	-36.526	0.0
E6	0.6293	0.053	11.983	0.0
Vkabat	0.0154	0.016	0.967	0.333

Table B.171: Fields: Triplet-Both: isSwitch - E20 + Residue Type

Field	Value
Accuracy:	84.17422867513612
Df Residuals:	13776
Df Model:	20
Date:	Thu Apr 04 16:28:58 PDT 2019
Pseudo R-squ.:	0.02012
Log-Likelihood:	-5228.2
LL-Null:	-5335.5
LLR p-value:	1.389E-34

Table B.172: Descriptors: Triplet-Both: isSwitch - E20 + Residue Type

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.7555	0.124	-22.215	0.0
Alanine (A)	0.4817	0.15	3.207	0.001
Arginine (R)	0.4322	0.163	2.655	0.008
Asparagine (N)	0.6082	0.166	3.669	0.0
Aspartic acid (D)	0.6594	0.154	4.277	0.0
Cysteine (C)	0.3492	0.273	1.281	0.2
Glutamine (Q)	0.6711	0.147	4.553	0.0
Glutamic acid (E)	0.6633	0.165	4.018	0.0
Glycine (G)	0.0586	0.168	0.348	0.728
Histidine (H)	0.419	0.199	2.102	0.036
Isoleucine (I)	0.1923	0.167	1.151	0.25
Leucine (L)	0.3571	0.145	2.456	0.014
Lysine (K)	0.7546	0.15	5.03	0.0
Methionine (M)	0.7313	0.197	3.718	0.0
Phenylalanine (F)	0.4551	0.175	2.594	0.009
Proline (P)	0.5216	0.174	3.003	0.003
Serine (S)	0.6922	0.152	4.557	0.0
Threonine (T)	0.3645	0.169	2.153	0.031
Tryptophan (W)	0.6574	0.255	2.579	0.01
Tyrosine (Y)	0.3407	0.178	1.919	0.055
E20	0.4186	0.036	11.629	0.0

Table B.173: Fields: Triplet-Both: isSwitch - E20 + isUnstruct

Field	Value
Accuracy:	84.17422867513612
Df Residuals:	13794
Df Model:	2
Date:	Thu Apr 04 16:28:58 PDT 2019
Pseudo R-squ.:	0.02967
Log-Likelihood:	-5177.2
LL-Null:	-5335.5
LLR p-value:	1.748E-69

Table B.174: Descriptors: Triplet-Both: isSwitch - E20 + isUnstruct

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.5628	0.049	-51.943	0.0
E20	0.3744	0.036	10.337	0.0
isUnstruct	1.2365	0.091	13.643	0.0

Table B.175: Fields: Triplet-Both: isSwitch - E20 + Vkabat

Field	Value
Accuracy:	84.17422867513612
Df Residuals:	13794
Df Model:	2
Date:	Thu Apr 04 16:28:58 PDT 2019
Pseudo R-squ.:	0.01344
Log-Likelihood:	-5263.8
LL-Null:	-5335.5
LLR p-value:	7.074E-32

Table B.176: Descriptors: Triplet-Both: isSwitch - E20 + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.33	0.064	-36.307	0.0
E20	0.4325	0.036	12.124	0.0
Vkabat	0.0106	0.016	0.665	0.506

Table B.177: Fields: Triplet-Both: isSwitch - isUnstruct + Vkabat

Field	Value
Accuracy:	84.17422867513612
Df Residuals:	13794
Df Model:	2
Date:	Thu Apr 04 16:28:58 PDT 2019
Pseudo R-squ.:	0.02031
Log-Likelihood:	-5227.2
LL-Null:	-5335.5
LLR p-value:	8.833E-48

Table B.178: Descriptors: Triplet-Both: isSwitch - isUnstruct + Vkabat

Name	**Beta**	**Std Err**	**Z-score**	**P-value**
Intercept	-2.3494	0.062	-37.902	0.0
isUnstruct	1.3658	0.09	15.258	0.0
Vkabat	0.0336	0.016	2.094	0.036

Table B.179: Fields: Triplet-Both: isSwitch - isUnstruct + Residue Type

Field	**Value**
Accuracy:	84.17422867513612
Df Residuals:	13776
Df Model:	20
Date:	Thu Apr 04 16:28:58 PDT 2019
Pseudo R-squ.:	0.02437
Log-Likelihood:	-5205.5
LL-Null:	-5335.5
LLR p-value:	1.064E-43

Table B.180: Descriptors: Triplet-Both: isSwitch - isUnstruct + Residue Type

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.6208	0.121	-21.706	0.0
Alanine (A)	0.425	0.151	2.823	0.005
Arginine (R)	0.3599	0.163	2.206	0.027
Asparagine (N)	0.5546	0.166	3.336	0.001
Aspartic acid (D)	0.6205	0.154	4.017	0.0
Cysteine (C)	0.4184	0.273	1.535	0.125
Glutamine (Q)	0.5466	0.148	3.691	0.0
Glutamic acid (E)	0.499	0.166	3.007	0.003
Glycine (G)	0.029	0.168	0.172	0.863
Histidine (H)	0.41	0.2	2.055	0.04
Isoleucine (I)	0.1875	0.167	1.121	0.262
Leucine (L)	0.2897	0.145	1.991	0.046
Lysine (K)	0.6132	0.151	4.067	0.0
Methionine (M)	0.4622	0.199	2.325	0.02
Phenylalanine (F)	0.4793	0.176	2.73	0.006
Proline (P)	0.3271	0.175	1.87	0.061
Serine (S)	0.5238	0.153	3.421	0.001
Threonine (T)	0.2929	0.17	1.726	0.084
Tryptophan (W)	0.6447	0.255	2.531	0.011
Tyrosine (Y)	0.3509	0.178	1.975	0.048
isUnstruct	1.2747	0.093	13.741	0.0

Table B.181: Fields: Triplet-Both: isSwitch - Vkabat + Residue Type

Field	Value
Accuracy:	84.17422867513612
Df Residuals:	13776
Df Model:	20
Date:	Thu Apr 04 16:28:58 PDT 2019
Pseudo R-squ.:	0.007885
Log-Likelihood:	-5293.4
LL-Null:	-5335.5
LLR p-value:	7.690E-10

Table B.182: Descriptors: Triplet-Both: isSwitch - Vkabat + Residue Type

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.4315	0.13	-18.763	0.0
Alanine (A)	0.5122	0.15	3.419	0.001
Arginine (R)	0.469	0.162	2.895	0.004
Asparagine (N)	0.6389	0.165	3.867	0.0
Aspartic acid (D)	0.7175	0.154	4.671	0.0
Cysteine (C)	0.3526	0.271	1.299	0.194
Glutamine (Q)	0.7015	0.147	4.776	0.0
Glutamic acid (E)	0.6716	0.164	4.083	0.0
Glycine (G)	0.0689	0.168	0.41	0.682
Histidine (H)	0.4316	0.199	2.173	0.03
Isoleucine (I)	0.1742	0.167	1.046	0.295
Leucine (L)	0.3068	0.145	2.117	0.034
Lysine (K)	0.7688	0.149	5.144	0.0
Methionine (M)	0.7173	0.196	3.663	0.0
Phenylalanine (F)	0.3958	0.175	2.265	0.024
Proline (P)	0.5513	0.174	3.175	0.001
Serine (S)	0.737	0.151	4.872	0.0
Threonine (T)	0.3862	0.169	2.291	0.022
Tryptophan (W)	0.5261	0.254	2.073	0.038
Tyrosine (Y)	0.2655	0.177	1.501	0.133
Vkabat	0.0191	0.016	1.186	0.236

Table B.183: Fields: Triplet-Both: isSwitch - E6 + isUnstruct + Vkabat

Field	Value
Accuracy:	84.17422867513612
Df Residuals:	13793
Df Model:	3
Date:	Thu Apr 04 16:28:59 PDT 2019
Pseudo R-squ.:	0.02896
Log-Likelihood:	-5181.0
LL-Null:	-5335.5
LLR p-value:	1.115E-66

Table B.184: Descriptors: Triplet-Both: isSwitch - E6 + isUnstruct + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.6096	0.069	-37.949	0.0
E6	0.5231	0.054	9.747	0.0
isUnstruct	1.2324	0.091	13.474	0.0
Vkabat	0.0355	0.016	2.205	0.027

Table B.185: Fields: Triplet-Both: isSwitch - E6 + Residue Type + Vkabat

Field	Value
Accuracy:	84.17422867513612
Df Residuals:	13775
Df Model:	21
Date:	Thu Apr 04 16:28:59 PDT 2019
Pseudo R-squ.:	0.01904
Log-Likelihood:	-5234.0
LL-Null:	-5335.5
LLR p-value:	8.758E-32

Table B.186: Descriptors: Triplet-Both: isSwitch - E6 + Residue Type + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.705	0.133	-20.331	0.0
Alanine (A)	0.4241	0.151	2.816	0.005
Arginine (R)	0.3674	0.163	2.255	0.024
Asparagine (N)	0.5503	0.166	3.312	0.001
Aspartic acid (D)	0.6008	0.155	3.883	0.0
Cysteine (C)	0.3035	0.273	1.114	0.265
Glutamine (Q)	0.6048	0.148	4.093	0.0
Glutamic acid (E)	0.5827	0.165	3.524	0.0
Glycine (G)	-0.009	0.169	-0.053	0.957
Histidine (H)	0.3573	0.2	1.791	0.073
Isoleucine (I)	0.1852	0.167	1.109	0.268
Leucine (L)	0.3233	0.145	2.225	0.026
Lysine (K)	0.6921	0.15	4.605	0.0
Methionine (M)	0.7236	0.197	3.682	0.0
Phenylalanine (F)	0.4023	0.175	2.295	0.022
Proline (P)	0.4445	0.175	2.543	0.011
Serine (S)	0.6301	0.152	4.139	0.0
Threonine (T)	0.3147	0.169	1.858	0.063
Tryptophan (W)	0.5716	0.255	2.245	0.025
Tyrosine (Y)	0.293	0.177	1.652	0.099
E6	0.5927	0.054	11.06	0.0
Vkabat	0.0205	0.016	1.265	0.206

Table B.187: Fields: Triplet-Both: isSwitch - E6 + Residue Type + isUnstruct

Field	Value
Accuracy:	84.17422867513612
Df Residuals:	13775
Df Model:	21
Date:	Thu Apr 04 16:28:59 PDT 2019
Pseudo R-squ.:	0.03243
Log-Likelihood:	-5162.5
LL-Null:	-5335.5
LLR p-value:	1.243E-60

Table B.188: Descriptors: Triplet-Both: isSwitch - E6 + Residue Type + isUnstruct

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.8315	0.123	-22.929	0.0
Alanine (A)	0.3542	0.151	2.343	0.019
Arginine (R)	0.2795	0.164	1.705	0.088
Asparagine (N)	0.4826	0.167	2.89	0.004
Aspartic acid (D)	0.5269	0.155	3.393	0.001
Cysteine (C)	0.3668	0.274	1.34	0.18
Glutamine (Q)	0.4793	0.149	3.225	0.001
Glutamic acid (E)	0.4433	0.166	2.664	0.008
Glycine (G)	-0.042	0.169	-0.248	0.804
Histidine (H)	0.342	0.201	1.705	0.088
Isoleucine (I)	0.1943	0.168	1.159	0.247
Leucine (L)	0.3016	0.146	2.067	0.039
Lysine (K)	0.5623	0.151	3.718	0.0
Methionine (M)	0.4929	0.199	2.477	0.013
Phenylalanine (F)	0.4777	0.176	2.715	0.007
Proline (P)	0.2508	0.176	1.428	0.153
Serine (S)	0.4457	0.154	2.897	0.004
Threonine (T)	0.2402	0.17	1.411	0.158
Tryptophan (W)	0.6725	0.255	2.632	0.008
Tyrosine (Y)	0.3675	0.178	2.064	0.039
E6	0.5115	0.054	9.388	0.0
isUnstruct	1.1651	0.094	12.375	0.0

Table B.189: Fields: Triplet-Both: isSwitch - E20 + isUnstruct + Vkabat

Field	Value
Accuracy:	84.17422867513612
Df Residuals:	13793
Df Model:	3
Date:	Thu Apr 04 16:28:59 PDT 2019
Pseudo R-squ.:	0.03002
Log-Likelihood:	-5175.3
LL-Null:	-5335.5
LLR p-value:	3.938E-69

Table B.190: Descriptors: Triplet-Both: isSwitch - E20 + isUnstruct + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.658	0.07	-37.888	0.0
E20	0.3731	0.036	10.303	0.0
isUnstruct	1.2543	0.091	13.767	0.0
Vkabat	0.0312	0.016	1.932	0.053

Table B.191: Fields: Triplet-Both: isSwitch - E20 + Residue Type + Vkabat

Field	Value
Accuracy:	84.17422867513612
Df Residuals:	13775
Df Model:	21
Date:	Thu Apr 04 16:29:00 PDT 2019
Pseudo R-squ.:	0.02022
Log-Likelihood:	-5227.6
LL-Null:	-5335.5
LLR p-value:	2.766E-34

Table B.192: Descriptors: Triplet-Both: isSwitch - E20 + Residue Type + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.8113	0.135	-20.857	0.0
Alanine (A)	0.49	0.15	3.257	0.001
Arginine (R)	0.433	0.163	2.66	0.008
Asparagine (N)	0.6167	0.166	3.715	0.0
Aspartic acid (D)	0.6684	0.154	4.328	0.0
Cysteine (C)	0.351	0.273	1.287	0.198
Glutamine (Q)	0.6778	0.148	4.594	0.0
Glutamic acid (E)	0.6704	0.165	4.057	0.0
Glycine (G)	0.0706	0.169	0.418	0.676
Histidine (H)	0.4209	0.199	2.111	0.035
Isoleucine (I)	0.1918	0.167	1.148	0.251
Leucine (L)	0.3624	0.145	2.491	0.013
Lysine (K)	0.7615	0.15	5.071	0.0
Methionine (M)	0.7362	0.197	3.742	0.0
Phenylalanine (F)	0.4557	0.175	2.597	0.009
Proline (P)	0.5387	0.174	3.087	0.002
Serine (S)	0.6971	0.152	4.586	0.0
Threonine (T)	0.3652	0.169	2.157	0.031
Tryptophan (W)	0.6559	0.255	2.573	0.01
Tyrosine (Y)	0.343	0.178	1.931	0.053
E20	0.418	0.036	11.616	0.0
Vkabat	0.0173	0.016	1.065	0.287

Table B.193: Fields: Triplet-Both: isSwitch - E20 + Residue Type + isUnstruct

Field	Value
Accuracy:	84.17422867513612
Df Residuals:	13775
Df Model:	21
Date:	Thu Apr 04 16:29:00 PDT 2019
Pseudo R-squ.:	0.034
Log-Likelihood:	-5154.1
LL-Null:	-5335.5
LLR p-value:	4.336E-64

Table B.194: Descriptors: Triplet-Both: isSwitch - E20 + Residue Type + isUnstruct

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.946	0.126	-23.417	0.0
Alanine (A)	0.4097	0.151	2.712	0.007
Arginine (R)	0.3325	0.164	2.03	0.042
Asparagine (N)	0.5379	0.167	3.222	0.001
Aspartic acid (D)	0.5824	0.155	3.755	0.0
Cysteine (C)	0.4082	0.274	1.491	0.136
Glutamine (Q)	0.5397	0.149	3.634	0.0
Glutamic acid (E)	0.5173	0.166	3.109	0.002
Glycine (G)	0.0285	0.169	0.169	0.866
Histidine (H)	0.3959	0.2	1.975	0.048
Isoleucine (I)	0.1987	0.168	1.184	0.236
Leucine (L)	0.337	0.146	2.308	0.021
Lysine (K)	0.6206	0.151	4.103	0.0
Methionine (M)	0.5023	0.199	2.521	0.012
Phenylalanine (F)	0.5259	0.176	2.986	0.003
Proline (P)	0.3321	0.175	1.892	0.058
Serine (S)	0.5002	0.154	3.254	0.001
Threonine (T)	0.2803	0.17	1.646	0.1
Tryptophan (W)	0.7499	0.256	2.932	0.003
Tyrosine (Y)	0.4137	0.178	2.321	0.02
E20	0.3738	0.036	10.254	0.0
isUnstruct	1.1789	0.094	12.537	0.0

Table B.195: Fields: Triplet-Both: isSwitch - Residue Type + isUnstruct + Vkabat

Field	Value
Accuracy:	84.17422867513612
Df Residuals:	13775
Df Model:	21
Date:	Thu Apr 04 16:29:00 PDT 2019
Pseudo R-squ.:	0.02486
Log-Likelihood:	-5202.9
LL-Null:	-5335.5
LLR p-value:	3.406E-44

Table B.196: Descriptors: Triplet-Both: isSwitch - Residue Type + isUnstruct + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.7487	0.133	-20.622	0.0
Alanine (A)	0.4433	0.151	2.939	0.003
Arginine (R)	0.3604	0.163	2.208	0.027
Asparagine (N)	0.5752	0.167	3.455	0.001
Aspartic acid (D)	0.6398	0.155	4.135	0.0
Cysteine (C)	0.4254	0.273	1.561	0.119
Glutamine (Q)	0.562	0.148	3.791	0.0
Glutamic acid (E)	0.5155	0.166	3.103	0.002
Glycine (G)	0.0567	0.169	0.336	0.737
Histidine (H)	0.4158	0.2	2.083	0.037
Isoleucine (I)	0.1861	0.167	1.112	0.266
Leucine (L)	0.3023	0.146	2.075	0.038
Lysine (K)	0.6275	0.151	4.157	0.0
Methionine (M)	0.4707	0.199	2.367	0.018
Phenylalanine (F)	0.4835	0.176	2.754	0.006
Proline (P)	0.3628	0.176	2.066	0.039
Serine (S)	0.5337	0.153	3.484	0.0
Threonine (T)	0.2937	0.17	1.73	0.084
Tryptophan (W)	0.6437	0.255	2.526	0.012
Tyrosine (Y)	0.3575	0.178	2.011	0.044
isUnstruct	1.293	0.093	13.891	0.0
Vkabat	0.0376	0.016	2.304	0.021

Table B.197: Fields: Triplet-Both: isSwitch - E6 + Residue Type + isUnstruct + Vkabat

Field	Value
Accuracy:	84.17422867513612
Df Residuals:	13774
Df Model:	22
Date:	Thu Apr 04 16:29:00 PDT 2019
Pseudo R-squ.:	0.03291
Log-Likelihood:	-5159.9
LL-Null:	-5335.5
LLR p-value:	4.395E-61

Table B.198: Descriptors: Triplet-Both: isSwitch - E6 + Residue Type + isUnstruct + Vkabat

Name	**Beta**	**Std Err**	**Z-score**	**P-value**
Intercept	-2.9604	0.136	-21.745	0.0
Alanine (A)	0.3737	0.152	2.467	0.014
Arginine (R)	0.2817	0.164	1.717	0.086
Asparagine (N)	0.5043	0.167	3.014	0.003
Aspartic acid (D)	0.5485	0.156	3.525	0.0
Cysteine (C)	0.3752	0.274	1.37	0.171
Glutamine (Q)	0.4953	0.149	3.328	0.001
Glutamic acid (E)	0.4608	0.167	2.766	0.006
Glycine (G)	-0.0116	0.17	-0.068	0.945
Histidine (H)	0.3492	0.201	1.741	0.082
Isoleucine (I)	0.1939	0.168	1.156	0.248
Leucine (L)	0.3147	0.146	2.155	0.031
Lysine (K)	0.5781	0.151	3.817	0.0
Methionine (M)	0.5026	0.199	2.524	0.012
Phenylalanine (F)	0.4826	0.176	2.741	0.006
Proline (P)	0.2883	0.176	1.634	0.102
Serine (S)	0.4572	0.154	2.97	0.003
Threonine (T)	0.2433	0.17	1.428	0.153
Tryptophan (W)	0.6734	0.256	2.635	0.008
Tyrosine (Y)	0.3757	0.178	2.109	0.035
E6	0.5112	0.054	9.386	0.0
isUnstruct	1.1839	0.094	12.53	0.0
Vkabat	0.0375	0.016	2.294	0.022

Table B.199: Fields: Triplet-Both: isSwitch - E20 + Residue Type + isUnstruct + Vkabat

Field	**Value**
Accuracy:	84.17422867513612
Df Residuals:	13774
Df Model:	22
Date:	Thu Apr 04 16:29:00 PDT 2019
Pseudo R-squ.:	0.03441
Log-Likelihood:	-5151.9
LL-Null:	-5335.5
LLR p-value:	2.303E-64

Table B.200: Descriptors: Triplet-Both: isSwitch - E20 + Residue Type + isUnstruct + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-3.062	0.138	-22.227	0.0
Alanine (A)	0.4268	0.151	2.819	0.005
Arginine (R)	0.3338	0.164	2.037	0.042
Asparagine (N)	0.5567	0.167	3.33	0.001
Aspartic acid (D)	0.6015	0.155	3.871	0.0
Cysteine (C)	0.4151	0.274	1.516	0.13
Glutamine (Q)	0.5536	0.149	3.723	0.0
Glutamic acid (E)	0.5323	0.167	3.195	0.001
Glycine (G)	0.0552	0.169	0.326	0.744
Histidine (H)	0.4017	0.201	2.003	0.045
Isoleucine (I)	0.1978	0.168	1.178	0.239
Leucine (L)	0.3482	0.146	2.382	0.017
Lysine (K)	0.6342	0.151	4.187	0.0
Methionine (M)	0.5104	0.199	2.561	0.01
Phenylalanine (F)	0.5295	0.176	3.005	0.003
Proline (P)	0.3657	0.176	2.075	0.038
Serine (S)	0.51	0.154	3.315	0.001
Threonine (T)	0.2822	0.17	1.657	0.098
Tryptophan (W)	0.7495	0.256	2.93	0.003
Tyrosine (Y)	0.4204	0.178	2.358	0.018
E20	0.372	0.036	10.209	0.0
isUnstruct	1.1961	0.094	12.675	0.0
Vkabat	0.0345	0.016	2.103	0.035

Table B.201: Fields: Triplet-Assigned: isSwitch - Residue Type

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13777
Df Model:	19
Date:	Thu Apr 04 16:28:50 PDT 2019
Pseudo R-squ.:	0.005799
Log-Likelihood:	-4187.2
LL-Null:	-4211.6
LLR p-value:	0.0001935

Table B.202: Descriptors: Triplet-Assigned: isSwitch - Residue Type

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.5673	0.129	-19.947	0.0
Alanine (A)	0.1842	0.171	1.079	0.281
Arginine (R)	0.3808	0.178	2.135	0.033
Asparagine (N)	0.3589	0.188	1.908	0.056
Aspartic acid (D)	0.4351	0.173	2.51	0.012
Cysteine (C)	0.1283	0.317	0.405	0.685
Glutamine (Q)	0.5342	0.162	3.293	0.001
Glutamic acid (E)	0.4745	0.184	2.579	0.01
Glycine (G)	-0.3602	0.201	-1.79	0.073
Histidine (H)	0.345	0.22	1.571	0.116
Isoleucine (I)	0.0797	0.184	0.432	0.666
Leucine (L)	0.1754	0.16	1.097	0.273
Lysine (K)	0.4458	0.169	2.636	0.008
Methionine (M)	0.3481	0.231	1.505	0.132
Phenylalanine (F)	0.4163	0.188	2.21	0.027
Proline (P)	0.2354	0.2	1.178	0.239
Serine (S)	0.3714	0.173	2.146	0.032
Threonine (T)	0.0556	0.197	0.283	0.777
Tryptophan (W)	0.5078	0.276	1.843	0.065
Tyrosine (Y)	0.2757	0.191	1.441	0.149

Table B.203: Fields: Triplet-Assigned: isSwitch - E6

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13795
Df Model:	1
Date:	Thu Apr 04 16:28:51 PDT 2019
Pseudo R-squ.:	0.004821
Log-Likelihood:	-4191.3
LL-Null:	-4211.6
LLR p-value:	1.858E-10

Table B.204: Descriptors: Triplet-Assigned: isSwitch - E6

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.5152	0.046	-54.385	0.0
E6	0.4016	0.062	6.478	0.0

Table B.205: Fields: Triplet-Assigned: isSwitch - E20

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13795
Df Model:	1
Date:	Thu Apr 04 16:28:51 PDT 2019
Pseudo R-squ.:	0.005291
Log-Likelihood:	-4189.4
LL-Null:	-4211.6
LLR p-value:	2.458E-11

Table B.206: Descriptors: Triplet-Assigned: isSwitch - E20

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.5562	0.05	-51.175	0.0
E20	0.2844	0.042	6.774	0.0

Table B.207: Fields: Triplet-Assigned: isSwitch - isUnstruct

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13795
Df Model:	1
Date:	Thu Apr 04 16:28:51 PDT 2019
Pseudo R-squ.:	7.535E-6
Log-Likelihood:	-4211.6
LL-Null:	-4211.6
LLR p-value:	0.8011

Table B.208: Descriptors: Triplet-Assigned: isSwitch - isUnstruct

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.2925	0.04	-57.319	0.0
isUnstruct	-0.0303	0.121	-0.252	0.801

Table B.209: Fields: Triplet-Assigned: isSwitch - Vkabat

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13795
Df Model:	1
Date:	Thu Apr 04 16:28:51 PDT 2019
Pseudo R-squ.:	0.00208
Log-Likelihood:	-4202.9
LL-Null:	-4211.6
LLR p-value:	0.00002848

Table B.210: Descriptors: Triplet-Assigned: isSwitch - Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.5291	0.063	-40.079	0.0
Vkabat	0.0761	0.018	4.234	0.0

Table B.211: Fields: Triplet-Assigned: isSwitch - E6 + Residue Type

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13776
Df Model:	20
Date:	Thu Apr 04 16:28:51 PDT 2019
Pseudo R-squ.:	0.01017
Log-Likelihood:	-4168.8
LL-Null:	-4211.6
LLR p-value:	4.134E-10

Table B.212: Descriptors: Triplet-Assigned: isSwitch - E6 + Residue Type

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.7385	0.132	-20.72	0.0
Alanine (A)	0.1245	0.171	0.728	0.467
Arginine (R)	0.3141	0.179	1.755	0.079
Asparagine (N)	0.2989	0.189	1.584	0.113
Aspartic acid (D)	0.3561	0.174	2.046	0.041
Cysteine (C)	0.0954	0.317	0.301	0.763
Glutamine (Q)	0.4695	0.163	2.884	0.004
Glutamic acid (E)	0.4145	0.185	2.247	0.025
Glycine (G)	-0.4124	0.202	-2.045	0.041
Histidine (H)	0.2955	0.22	1.343	0.179
Isoleucine (I)	0.0857	0.185	0.464	0.642
Leucine (L)	0.1846	0.16	1.153	0.249
Lysine (K)	0.3927	0.17	2.316	0.021
Methionine (M)	0.3487	0.232	1.506	0.132
Phenylalanine (F)	0.4194	0.189	2.224	0.026
Proline (P)	0.1634	0.2	0.815	0.415
Serine (S)	0.2986	0.174	1.719	0.086
Threonine (T)	0.0075	0.197	0.038	0.97
Tryptophan (W)	0.5352	0.276	1.94	0.052
Tyrosine (Y)	0.2918	0.191	1.524	0.128
E6	0.3898	0.063	6.158	0.0

Table B.213: Fields: Triplet-Assigned: isSwitch - E6 + isUnstruct

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13794
Df Model:	2
Date:	Thu Apr 04 16:28:51 PDT 2019
Pseudo R-squ.:	0.005033
Log-Likelihood:	-4190.4
LL-Null:	-4211.6
LLR p-value:	6.221E-10

Table B.214: Descriptors: Triplet-Assigned: isSwitch - E6 + isUnstruct

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.4863	0.051	-48.777	0.0
E6	0.4159	0.063	6.613	0.0
isUnstruct	-0.1637	0.124	-1.325	0.185

Table B.215: Fields: Triplet-Assigned: isSwitch - E6 + Vkabat

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13794
Df Model:	2
Date:	Thu Apr 04 16:28:51 PDT 2019
Pseudo R-squ.:	0.007041
Log-Likelihood:	-4182.0
LL-Null:	-4211.6
LLR p-value:	1.320E-13

Table B.216: Descriptors: Triplet-Assigned: isSwitch - E6 + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.7563	0.073	-37.671	0.0
E6	0.4078	0.062	6.572	0.0
Vkabat	0.0788	0.018	4.376	0.0

Table B.217: Fields: Triplet-Assigned: isSwitch - E20 + Residue Type

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13776
Df Model:	20
Date:	Thu Apr 04 16:28:52 PDT 2019
Pseudo R-squ.:	0.01091
Log-Likelihood:	-4165.7
LL-Null:	-4211.6
LLR p-value:	3.426E-11

Table B.218: Descriptors: Triplet-Assigned: isSwitch - E20 + Residue Type

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.821	0.135	-20.898	0.0
Alanine (A)	0.1681	0.171	0.984	0.325
Arginine (R)	0.3563	0.179	1.994	0.046
Asparagine (N)	0.3429	0.188	1.82	0.069
Aspartic acid (D)	0.4003	0.174	2.304	0.021
Cysteine (C)	0.1267	0.317	0.4	0.69
Glutamine (Q)	0.5176	0.162	3.185	0.001
Glutamic acid (E)	0.4727	0.184	2.565	0.01
Glycine (G)	-0.3594	0.201	-1.784	0.074
Histidine (H)	0.3368	0.22	1.531	0.126
Isoleucine (I)	0.0906	0.185	0.491	0.624
Leucine (L)	0.2121	0.16	1.324	0.186
Lysine (K)	0.4388	0.169	2.59	0.01
Methionine (M)	0.358	0.232	1.545	0.122
Phenylalanine (F)	0.4556	0.189	2.414	0.016
Proline (P)	0.2265	0.2	1.132	0.258
Serine (S)	0.3421	0.173	1.973	0.048
Threonine (T)	0.0403	0.197	0.205	0.838
Tryptophan (W)	0.592	0.276	2.144	0.032
Tyrosine (Y)	0.3262	0.192	1.702	0.089
E20	0.2817	0.042	6.653	0.0

Table B.219: Fields: Triplet-Assigned: isSwitch - E20 + isUnstruct

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13794
Df Model:	2
Date:	Thu Apr 04 16:28:52 PDT 2019
Pseudo R-squ.:	0.005452
Log-Likelihood:	-4188.7
LL-Null:	-4211.6
LLR p-value:	1.065E-10

Table B.220: Descriptors: Triplet-Assigned: isSwitch - E20 + isUnstruct

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.5306	0.054	-46.442	0.0
E20	0.2913	0.042	6.87	0.0
isUnstruct	-0.1422	0.123	-1.157	0.247

Table B.221: Fields: Triplet-Assigned: isSwitch - E20 + Vkabat

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13794
Df Model:	2
Date:	Thu Apr 04 16:28:52 PDT 2019
Pseudo R-squ.:	0.007355
Log-Likelihood:	-4180.7
LL-Null:	-4211.6
LLR p-value:	3.529E-14

Table B.222: Descriptors: Triplet-Assigned: isSwitch - E20 + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.7847	0.075	-37.227	0.0
E20	0.2836	0.042	6.764	0.0
Vkabat	0.076	0.018	4.218	0.0

Table B.223: Fields: Triplet-Assigned: isSwitch - isUnstruct + Vkabat

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13794
Df Model:	2
Date:	Thu Apr 04 16:28:52 PDT 2019
Pseudo R-squ.:	0.002082
Log-Likelihood:	-4202.9
LL-Null:	-4211.6
LLR p-value:	0.0001558

Table B.224: Descriptors: Triplet-Assigned: isSwitch - isUnstruct + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.5334	0.071	-35.756	0.0
isUnstruct	0.0158	0.121	0.131	0.896
Vkabat	0.0764	0.018	4.228	0.0

Table B.225: Fields: Triplet-Assigned: isSwitch - isUnstruct + Residue Type

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13776
Df Model:	20
Date:	Thu Apr 04 16:28:52 PDT 2019
Pseudo R-squ.:	0.005919
Log-Likelihood:	-4186.7
LL-Null:	-4211.6
LLR p-value:	0.0002321

Table B.226: Descriptors: Triplet-Assigned: isSwitch - isUnstruct + Residue Type

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.5462	0.13	-19.528	0.0
Alanine (A)	0.1915	0.171	1.121	0.262
Arginine (R)	0.3909	0.179	2.189	0.029
Asparagine (N)	0.3657	0.188	1.943	0.052
Aspartic acid (D)	0.4437	0.174	2.557	0.011
Cysteine (C)	0.123	0.317	0.389	0.698
Glutamine (Q)	0.5479	0.163	3.366	0.001
Glutamic acid (E)	0.4896	0.185	2.653	0.008
Glycine (G)	-0.3576	0.201	-1.777	0.076
Histidine (H)	0.3476	0.22	1.583	0.114
Isoleucine (I)	0.0789	0.184	0.428	0.669
Leucine (L)	0.1768	0.16	1.105	0.269
Lysine (K)	0.4593	0.17	2.707	0.007
Methionine (M)	0.3698	0.232	1.592	0.111
Phenylalanine (F)	0.4099	0.188	2.174	0.03
Proline (P)	0.2539	0.201	1.266	0.206
Serine (S)	0.3904	0.174	2.243	0.025
Threonine (T)	0.064	0.197	0.325	0.745
Tryptophan (W)	0.4986	0.276	1.809	0.07
Tyrosine (Y)	0.2689	0.191	1.405	0.16
isUnstruct	-0.1253	0.125	-1.001	0.317

Table B.227: Fields: Triplet-Assigned: isSwitch - Vkabat + Residue Type

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13776
Df Model:	20
Date:	Thu Apr 04 16:28:52 PDT 2019
Pseudo R-squ.:	0.007938
Log-Likelihood:	-4178.2
LL-Null:	-4211.6
LLR p-value:	5.877E-7

Table B.228: Descriptors: Triplet-Assigned: isSwitch - Vkabat + Residue Type

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.8271	0.143	-19.762	0.0
Alanine (A)	0.221	0.171	1.292	0.196
Arginine (R)	0.3823	0.178	2.142	0.032
Asparagine (N)	0.3988	0.188	2.116	0.034
Aspartic acid (D)	0.4737	0.174	2.727	0.006
Cysteine (C)	0.1348	0.317	0.426	0.67
Glutamine (Q)	0.5661	0.163	3.483	0.0
Glutamic acid (E)	0.5075	0.184	2.754	0.006
Glycine (G)	-0.3092	0.202	-1.533	0.125
Histidine (H)	0.3526	0.22	1.604	0.109
Isoleucine (I)	0.0765	0.185	0.415	0.679
Leucine (L)	0.1995	0.16	1.246	0.213
Lysine (K)	0.4769	0.169	2.815	0.005
Methionine (M)	0.3696	0.232	1.596	0.11
Phenylalanine (F)	0.4203	0.189	2.23	0.026
Proline (P)	0.3124	0.201	1.556	0.12
Serine (S)	0.3922	0.173	2.263	0.024
Threonine (T)	0.0548	0.197	0.278	0.781
Tryptophan (W)	0.4988	0.276	1.809	0.07
Tyrosine (Y)	0.2849	0.191	1.488	0.137
Vkabat	0.0783	0.018	4.293	0.0

Table B.229: Fields: Triplet-Assigned: isSwitch - E6 + isUnstruct + Vkabat

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13793
Df Model:	3
Date:	Thu Apr 04 16:28:53 PDT 2019
Pseudo R-squ.:	0.007146
Log-Likelihood:	-4181.5
LL-Null:	-4211.6
LLR p-value:	5.338E-13

Table B.230: Descriptors: Triplet-Assigned: isSwitch - E6 + isUnstruct + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.7308	0.078	-35.043	0.0
E6	0.4177	0.063	6.639	0.0
isUnstruct	-0.1158	0.124	-0.935	0.35
Vkabat	0.0772	0.018	4.268	0.0

Table B.231: Fields: Triplet-Assigned: isSwitch - E6 + Residue Type + Vkabat

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13775
Df Model:	21
Date:	Thu Apr 04 16:28:53 PDT 2019
Pseudo R-squ.:	0.01234
Log-Likelihood:	-4159.7
LL-Null:	-4211.6
LLR p-value:	5.833E-13

Table B.232: Descriptors: Triplet-Assigned: isSwitch - E6 + Residue Type + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-3.0029	0.147	-20.476	0.0
Alanine (A)	0.1639	0.171	0.956	0.339
Arginine (R)	0.3185	0.179	1.779	0.075
Asparagine (N)	0.3413	0.189	1.806	0.071
Aspartic acid (D)	0.3993	0.174	2.289	0.022
Cysteine (C)	0.1048	0.317	0.331	0.741
Glutamine (Q)	0.5029	0.163	3.082	0.002
Glutamic acid (E)	0.4497	0.185	2.433	0.015
Glycine (G)	-0.3555	0.202	-1.758	0.079
Histidine (H)	0.3061	0.22	1.39	0.165
Isoleucine (I)	0.0844	0.185	0.457	0.648
Leucine (L)	0.2103	0.16	1.311	0.19
Lysine (K)	0.4267	0.17	2.512	0.012
Methionine (M)	0.3727	0.232	1.607	0.108
Phenylalanine (F)	0.4249	0.189	2.251	0.024
Proline (P)	0.2445	0.201	1.214	0.225
Serine (S)	0.3231	0.174	1.858	0.063
Threonine (T)	0.0111	0.197	0.056	0.955
Tryptophan (W)	0.5297	0.276	1.918	0.055
Tyrosine (Y)	0.3041	0.192	1.587	0.113
E6	0.3906	0.063	6.173	0.0
Vkabat	0.0788	0.018	4.315	0.0

Table B.233: Fields: Triplet-Assigned: isSwitch - E6 + Residue Type + isUnstruct

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13775
Df Model:	21
Date:	Thu Apr 04 16:28:53 PDT 2019
Pseudo R-squ.:	0.01058
Log-Likelihood:	-4167.1
LL-Null:	-4211.6
LLR p-value:	2.316E-10

Table B.234: Descriptors: Triplet-Assigned: isSwitch - E6 + Residue Type + isUnstruct

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.7064	0.133	-20.305	0.0
Alanine (A)	0.1357	0.171	0.793	0.428
Arginine (R)	0.3303	0.179	1.843	0.065
Asparagine (N)	0.3092	0.189	1.638	0.101
Aspartic acid (D)	0.3686	0.174	2.116	0.034
Cysteine (C)	0.0847	0.317	0.267	0.789
Glutamine (Q)	0.4915	0.163	3.011	0.003
Glutamic acid (E)	0.4387	0.185	2.371	0.018
Glycine (G)	-0.4091	0.202	-2.028	0.043
Histidine (H)	0.299	0.22	1.359	0.174
Isoleucine (I)	0.0846	0.185	0.458	0.647
Leucine (L)	0.1879	0.16	1.174	0.241
Lysine (K)	0.4149	0.17	2.44	0.015
Methionine (M)	0.388	0.233	1.668	0.095
Phenylalanine (F)	0.4076	0.189	2.16	0.031
Proline (P)	0.1946	0.201	0.968	0.333
Serine (S)	0.3312	0.175	1.897	0.058
Threonine (T)	0.0209	0.197	0.106	0.916
Tryptophan (W)	0.5195	0.276	1.882	0.06
Tyrosine (Y)	0.2797	0.192	1.46	0.144
E6	0.4058	0.064	6.354	0.0
isUnstruct	-0.2317	0.127	-1.819	0.069

Table B.235: Fields: Triplet-Assigned: isSwitch - E20 + isUnstruct + Vkabat

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13793
Df Model:	3
Date:	Thu Apr 04 16:28:53 PDT 2019
Pseudo R-squ.:	0.007427
Log-Likelihood:	-4180.4
LL-Null:	-4211.6
LLR p-value:	1.665E-13

Table B.236: Descriptors: Triplet-Assigned: isSwitch - E20 + isUnstruct + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.7634	0.08	-34.738	0.0
E20	0.2883	0.042	6.806	0.0
isUnstruct	-0.096	0.123	-0.779	0.436
Vkabat	0.0746	0.018	4.125	0.0

Table B.237: Fields: Triplet-Assigned: isSwitch - E20 + Residue Type + Vkabat

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13775
Df Model:	21
Date:	Thu Apr 04 16:28:53 PDT 2019
Pseudo R-squ.:	0.01298
Log-Likelihood:	-4157.0
LL-Null:	-4211.6
LLR p-value:	6.314E-14

Table B.238: Descriptors: Triplet-Assigned: isSwitch - E20 + Residue Type + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-3.0752	0.149	-20.682	0.0
Alanine (A)	0.2049	0.171	1.197	0.231
Arginine (R)	0.3592	0.179	2.009	0.045
Asparagine (N)	0.3824	0.189	2.026	0.043
Aspartic acid (D)	0.4414	0.174	2.536	0.011
Cysteine (C)	0.1345	0.317	0.424	0.671
Glutamine (Q)	0.5487	0.163	3.37	0.001
Glutamic acid (E)	0.5052	0.185	2.737	0.006
Glycine (G)	-0.3059	0.202	-1.515	0.13
Histidine (H)	0.3454	0.22	1.569	0.117
Isoleucine (I)	0.0882	0.185	0.477	0.633
Leucine (L)	0.2355	0.16	1.468	0.142
Lysine (K)	0.4703	0.17	2.771	0.006
Methionine (M)	0.38	0.232	1.639	0.101
Phenylalanine (F)	0.459	0.189	2.43	0.015
Proline (P)	0.3043	0.201	1.513	0.13
Serine (S)	0.3644	0.174	2.099	0.036
Threonine (T)	0.0421	0.197	0.214	0.831
Tryptophan (W)	0.5844	0.276	2.114	0.034
Tyrosine (Y)	0.3367	0.192	1.755	0.079
E20	0.2792	0.042	6.602	0.0
Vkabat	0.077	0.018	4.216	0.0

Table B.239: Fields: Triplet-Assigned: isSwitch - E20 + Residue Type + isUnstruct

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13775
Df Model:	21
Date:	Thu Apr 04 16:28:53 PDT 2019
Pseudo R-squ.:	0.01128
Log-Likelihood:	-4164.1
LL-Null:	-4211.6
LLR p-value:	2.171E-11

Table B.240: Descriptors: Triplet-Assigned: isSwitch - E20 + Residue Type + isUnstruct

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.7916	0.136	-20.527	0.0
Alanine (A)	0.1809	0.171	1.057	0.29
Arginine (R)	0.3739	0.179	2.089	0.037
Asparagine (N)	0.355	0.189	1.883	0.06
Aspartic acid (D)	0.4146	0.174	2.384	0.017
Cysteine (C)	0.1178	0.317	0.371	0.71
Glutamine (Q)	0.5409	0.163	3.317	0.001
Glutamic acid (E)	0.4984	0.185	2.696	0.007
Glycine (G)	-0.3542	0.202	-1.758	0.079
Histidine (H)	0.342	0.22	1.555	0.12
Isoleucine (I)	0.0899	0.185	0.487	0.626
Leucine (L)	0.2162	0.16	1.349	0.177
Lysine (K)	0.462	0.17	2.719	0.007
Methionine (M)	0.3959	0.233	1.701	0.089
Phenylalanine (F)	0.4456	0.189	2.36	0.018
Proline (P)	0.259	0.201	1.289	0.197
Serine (S)	0.3754	0.174	2.152	0.031
Threonine (T)	0.0549	0.197	0.279	0.781
Tryptophan (W)	0.5786	0.276	2.094	0.036
Tyrosine (Y)	0.3157	0.192	1.646	0.1
E20	0.2904	0.043	6.812	0.0
isUnstruct	-0.2216	0.127	-1.743	0.081

Table B.241: Fields: Triplet-Assigned: isSwitch - Residue Type + isUnstruct + Vkabat

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13775
Df Model:	21
Date:	Thu Apr 04 16:28:54 PDT 2019
Pseudo R-squ.:	0.007991
Log-Likelihood:	-4178.0
LL-Null:	-4211.6
LLR p-value:	9.406E-7

Table B.242: Descriptors: Triplet-Assigned: isSwitch - Residue Type + isUnstruct + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.8093	0.145	-19.319	0.0
Alanine (A)	0.2252	0.171	1.316	0.188
Arginine (R)	0.3889	0.179	2.176	0.03
Asparagine (N)	0.4024	0.189	2.134	0.033
Aspartic acid (D)	0.4785	0.174	2.753	0.006
Cysteine (C)	0.1307	0.317	0.413	0.68
Glutamine (Q)	0.5745	0.163	3.525	0.0
Glutamic acid (E)	0.5168	0.185	2.797	0.005
Glycine (G)	-0.3086	0.202	-1.53	0.126
Histidine (H)	0.3539	0.22	1.61	0.107
Isoleucine (I)	0.076	0.185	0.412	0.681
Leucine (L)	0.2	0.16	1.249	0.212
Lysine (K)	0.4853	0.17	2.857	0.004
Methionine (M)	0.3836	0.232	1.65	0.099
Phenylalanine (F)	0.4157	0.189	2.204	0.028
Proline (P)	0.3234	0.201	1.606	0.108
Serine (S)	0.4042	0.174	2.32	0.02
Threonine (T)	0.0601	0.197	0.306	0.76
Tryptophan (W)	0.4926	0.276	1.785	0.074
Tyrosine (Y)	0.28	0.192	1.462	0.144
isUnstruct	-0.0841	0.125	-0.671	0.502
Vkabat	0.0773	0.018	4.225	0.0

Table B.243: Fields: Triplet-Assigned: isSwitch - E6 + Residue Type + isUnstruct + Vkabat

Field	Value
Accuracy:	92.8130671506352
Df Residuals:	13774
Df Model:	22
Date:	Thu Apr 04 16:28:54 PDT 2019
Pseudo R-squ.:	0.0126
Log-Likelihood:	-4158.6
LL-Null:	-4211.6
LLR p-value:	5.333E-13

Table B.244: Descriptors: Triplet-Assigned: isSwitch - E6 + Residue Type + isUnstruct + Vkabat

Name	**Beta**	**Std Err**	**Z-score**	**P-value**
Intercept	-2.9684	0.148	-20.013	0.0
Alanine (A)	0.1715	0.172	0.999	0.318
Arginine (R)	0.3314	0.179	1.849	0.064
Asparagine (N)	0.3476	0.189	1.839	0.066
Aspartic acid (D)	0.4076	0.175	2.335	0.02
Cysteine (C)	0.0951	0.317	0.3	0.764
Glutamine (Q)	0.5191	0.164	3.175	0.001
Glutamic acid (E)	0.4675	0.185	2.524	0.012
Glycine (G)	-0.3554	0.202	-1.758	0.079
Histidine (H)	0.308	0.22	1.398	0.162
Isoleucine (I)	0.0836	0.185	0.452	0.651
Leucine (L)	0.212	0.16	1.322	0.186
Lysine (K)	0.4435	0.17	2.604	0.009
Methionine (M)	0.4035	0.233	1.733	0.083
Phenylalanine (F)	0.4147	0.189	2.195	0.028
Proline (P)	0.267	0.202	1.322	0.186
Serine (S)	0.3481	0.175	1.993	0.046
Threonine (T)	0.0214	0.197	0.108	0.914
Tryptophan (W)	0.5167	0.276	1.871	0.061
Tyrosine (Y)	0.2936	0.192	1.531	0.126
E6	0.4036	0.064	6.321	0.0
isUnstruct	-0.1892	0.128	-1.484	0.138
Vkabat	0.0765	0.018	4.176	0.0

Table B.245: Fields: Triplet-Assigned: isSwitch - E20 + Residue Type + isUnstruct + Vkabat

Field	**Value**
Accuracy:	92.8130671506352
Df Residuals:	13774
Df Model:	22
Date:	Thu Apr 04 16:28:54 PDT 2019
Pseudo R-squ.:	0.01322
Log-Likelihood:	-4156.0
LL-Null:	-4211.6
LLR p-value:	6.359E-14

Table B.246: Descriptors: Triplet-Assigned: isSwitch - E20 + Residue Type + isUnstruct + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-3.0435	0.15	-20.261	0.0
Alanine (A)	0.2138	0.171	1.248	0.212
Arginine (R)	0.3732	0.179	2.084	0.037
Asparagine (N)	0.3903	0.189	2.066	0.039
Aspartic acid (D)	0.4511	0.174	2.59	0.01
Cysteine (C)	0.1263	0.317	0.398	0.691
Glutamine (Q)	0.566	0.163	3.467	0.001
Glutamic acid (E)	0.5243	0.185	2.832	0.005
Glycine (G)	-0.3042	0.202	-1.506	0.132
Histidine (H)	0.3487	0.22	1.584	0.113
Isoleucine (I)	0.0877	0.185	0.475	0.635
Leucine (L)	0.2379	0.16	1.482	0.138
Lysine (K)	0.4879	0.17	2.868	0.004
Methionine (M)	0.4097	0.233	1.759	0.079
Phenylalanine (F)	0.4503	0.189	2.383	0.017
Proline (P)	0.3278	0.202	1.625	0.104
Serine (S)	0.39	0.174	2.235	0.025
Threonine (T)	0.0533	0.197	0.27	0.787
Tryptophan (W)	0.5734	0.277	2.073	0.038
Tyrosine (Y)	0.3275	0.192	1.706	0.088
E20	0.2864	0.043	6.724	0.0
isUnstruct	-0.1804	0.127	-1.417	0.156
Vkabat	0.0749	0.018	4.083	0.0

Table B.247: Fields: Triplet-Unassigned: isSwitch - Residue Type

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13777
Df Model:	19
Date:	Thu Apr 04 16:29:03 PDT 2019
Pseudo R-squ.:	0.01934
Log-Likelihood:	-2228.9
LL-Null:	-2272.8
LLR p-value:	7.686E-11

Table B.248: Descriptors: Triplet-Unassigned: isSwitch - Residue Type

Name	Beta	Std Err	Z-score	P-value
Intercept	-4.2363	0.279	-15.165	0.0
Alanine (A)	1.2816	0.314	4.08	0.0
Arginine (R)	0.7269	0.356	2.039	0.041
Asparagine (N)	1.2989	0.336	3.862	0.0
Aspartic acid (D)	1.366	0.321	4.252	0.0
Cysteine (C)	0.9782	0.501	1.952	0.051
Glutamine (Q)	1.1071	0.321	3.451	0.001
Glutamic acid (E)	1.1558	0.344	3.361	0.001
Glycine (G)	1.0389	0.33	3.152	0.002
Histidine (H)	0.6867	0.425	1.615	0.106
Isoleucine (I)	0.51	0.363	1.404	0.16
Leucine (L)	0.7035	0.321	2.191	0.028
Lysine (K)	1.4819	0.314	4.722	0.0
Methionine (M)	1.5213	0.366	4.154	0.0
Phenylalanine (F)	0.2182	0.424	0.514	0.607
Proline (P)	1.2699	0.344	3.689	0.0
Serine (S)	1.5321	0.314	4.88	0.0
Threonine (T)	1.203	0.336	3.579	0.0
Tryptophan (W)	0.5228	0.578	0.904	0.366
Tyrosine (Y)	0.1605	0.424	0.379	0.705

Table B.249: Fields: Triplet-Unassigned: isSwitch - E6

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13795
Df Model:	1
Date:	Thu Apr 04 16:29:03 PDT 2019
Pseudo R-squ.:	0.0255
Log-Likelihood:	-2214.9
LL-Null:	-2272.8
LLR p-value:	5.018E-27

Table B.250: Descriptors: Triplet-Unassigned: isSwitch - E6

Name	Beta	Std Err	Z-score	P-value
Intercept	-3.7797	0.075	-50.284	0.0
E6	0.9563	0.086	11.11	0.0

Table B.251: Fields: Triplet-Unassigned: isSwitch - E20

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13795
Df Model:	1
Date:	Thu Apr 04 16:29:03 PDT 2019
Pseudo R-squ.:	0.02508
Log-Likelihood:	-2215.8
LL-Null:	-2272.8
LLR p-value:	1.294E-26

Table B.252: Descriptors: Triplet-Unassigned: isSwitch - E20

Name	Beta	Std Err	Z-score	P-value
Intercept	-3.8473	0.081	-47.643	0.0
E20	0.6464	0.059	10.973	0.0

Table B.253: Fields: Triplet-Unassigned: isSwitch - isUnstruct

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13795
Df Model:	1
Date:	Thu Apr 04 16:29:03 PDT 2019
Pseudo R-squ.:	0.1185
Log-Likelihood:	-2003.5
LL-Null:	-2272.8
LLR p-value:	3.552E-119

Table B.254: Descriptors: Triplet-Unassigned: isSwitch - isUnstruct

Name	Beta	Std Err	Z-score	P-value
Intercept	-4.3158	0.079	-54.549	0.0
isUnstruct	3.2374	0.135	23.957	0.0

Table B.255: Fields: Triplet-Unassigned: isSwitch - Vkabat

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13795
Df Model:	1
Date:	Thu Apr 04 16:29:03 PDT 2019
Pseudo R-squ.:	0.005996
Log-Likelihood:	-2259.2
LL-Null:	-2272.8
LLR p-value:	1.782E-7

Table B.256: Descriptors: Triplet-Unassigned: isSwitch - Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-2.7771	0.091	-30.461	0.0
Vkabat	-0.1543	0.031	-5.047	0.0

Table B.257: Fields: Triplet-Unassigned: isSwitch - E6 + Residue Type

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13776
Df Model:	20
Date:	Thu Apr 04 16:29:03 PDT 2019
Pseudo R-squ.:	0.03989
Log-Likelihood:	-2182.2
LL-Null:	-2272.8
LLR p-value:	5.301E-28

Table B.258: Descriptors: Triplet-Unassigned: isSwitch - E6 + Residue Type

Name	Beta	Std Err	Z-score	P-value
Intercept	-4.6584	0.284	-16.402	0.0
Alanine (A)	1.1431	0.315	3.628	0.0
Arginine (R)	0.5589	0.358	1.562	0.118
Asparagine (N)	1.1544	0.338	3.42	0.001
Aspartic acid (D)	1.1767	0.323	3.647	0.0
Cysteine (C)	0.8955	0.503	1.781	0.075
Glutamine (Q)	0.9472	0.322	2.942	0.003
Glutamic acid (E)	1.0112	0.345	2.931	0.003
Glycine (G)	0.9138	0.331	2.764	0.006
Histidine (H)	0.5655	0.426	1.326	0.185
Isoleucine (I)	0.5263	0.364	1.447	0.148
Leucine (L)	0.7276	0.322	2.262	0.024
Lysine (K)	1.3544	0.315	4.301	0.0
Methionine (M)	1.5304	0.367	4.167	0.0
Phenylalanine (F)	0.2239	0.425	0.527	0.598
Proline (P)	1.0954	0.346	3.168	0.002
Serine (S)	1.3625	0.315	4.323	0.0
Threonine (T)	1.0863	0.337	3.222	0.001
Tryptophan (W)	0.5892	0.579	1.018	0.309
Tyrosine (Y)	0.2014	0.424	0.474	0.635
E6	0.8705	0.088	9.907	0.0

Table B.259: Fields: Triplet-Unassigned: isSwitch - E6 + isUnstruct

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13794
Df Model:	2
Date:	Thu Apr 04 16:29:03 PDT 2019
Pseudo R-squ.:	0.1308
Log-Likelihood:	-1975.5
LL-Null:	-2272.8
LLR p-value:	7.542E-130

Table B.260: Descriptors: Triplet-Unassigned: isSwitch - E6 + isUnstruct

Name	Beta	Std Err	Z-score	P-value
Intercept	-4.6924	0.098	-47.882	0.0
E6	0.6939	0.091	7.615	0.0
isUnstruct	3.1087	0.138	22.576	0.0

Table B.261: Fields: Triplet-Unassigned: isSwitch - E6 + Vkabat

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13794
Df Model:	2
Date:	Thu Apr 04 16:29:03 PDT 2019
Pseudo R-squ.:	0.03102
Log-Likelihood:	-2202.3
LL-Null:	-2272.8
LLR p-value:	2.428E-31

Table B.262: Descriptors: Triplet-Unassigned: isSwitch - E6 + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-3.3636	0.11	-30.451	0.0
E6	0.9487	0.086	11.001	0.0
Vkabat	-0.1486	0.031	-4.85	0.0

Table B.263: Fields: Triplet-Unassigned: isSwitch - E20 + Residue Type

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13776
Df Model:	20
Date:	Thu Apr 04 16:29:04 PDT 2019
Pseudo R-squ.:	0.04124
Log-Likelihood:	-2179.1
LL-Null:	-2272.8
LLR p-value:	3.345E-29

Table B.264: Descriptors: Triplet-Unassigned: isSwitch - E20 + Residue Type

Name	Beta	Std Err	Z-score	P-value
Intercept	-4.8271	0.287	-16.802	0.0
Alanine (A)	1.2457	0.315	3.957	0.0
Arginine (R)	0.6605	0.357	1.848	0.065
Asparagine (N)	1.2585	0.337	3.731	0.0
Aspartic acid (D)	1.2836	0.322	3.984	0.0
Cysteine (C)	0.9676	0.503	1.925	0.054
Glutamine (Q)	1.0604	0.322	3.298	0.001
Glutamic acid (E)	1.1445	0.345	3.32	0.001
Glycine (G)	1.0423	0.33	3.156	0.002
Histidine (H)	0.6658	0.426	1.562	0.118
Isoleucine (I)	0.5352	0.364	1.471	0.141
Leucine (L)	0.7843	0.322	2.437	0.015
Lysine (K)	1.4604	0.315	4.641	0.0
Methionine (M)	1.5467	0.367	4.209	0.0
Phenylalanine (F)	0.3018	0.425	0.71	0.477
Proline (P)	1.2448	0.345	3.606	0.0
Serine (S)	1.4668	0.315	4.66	0.0
Threonine (T)	1.1637	0.337	3.453	0.001
Tryptophan (W)	0.7147	0.579	1.234	0.217
Tyrosine (Y)	0.2741	0.425	0.645	0.519
E20	0.6057	0.059	10.213	0.0

Table B.265: Fields: Triplet-Unassigned: isSwitch - E20 + isUnstruct

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13794
Df Model:	2
Date:	Thu Apr 04 16:29:04 PDT 2019
Pseudo R-squ.:	0.1331
Log-Likelihood:	-1970.3
LL-Null:	-2272.8
LLR p-value:	4.300E-132

Table B.266: Descriptors: Triplet-Unassigned: isSwitch - E20 + isUnstruct

Name	Beta	Std Err	Z-score	P-value
Intercept	-4.7923	0.103	-46.352	0.0
E20	0.5079	0.061	8.277	0.0
isUnstruct	3.1431	0.138	22.852	0.0

Table B.267: Fields: Triplet-Unassigned: isSwitch - E20 + Vkabat

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13794
Df Model:	2
Date:	Thu Apr 04 16:29:04 PDT 2019
Pseudo R-squ.:	0.03134
Log-Likelihood:	-2201.6
LL-Null:	-2272.8
LLR p-value:	1.169E-31

Table B.268: Descriptors: Triplet-Unassigned: isSwitch - E20 + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-3.4163	0.113	-30.272	0.0
E20	0.6533	0.059	11.026	0.0
Vkabat	-0.1583	0.031	-5.152	0.0

Table B.269: Fields: Triplet-Unassigned: isSwitch - isUnstruct + Vkabat

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13794
Df Model:	2
Date:	Thu Apr 04 16:29:04 PDT 2019
Pseudo R-squ.:	0.1207
Log-Likelihood:	-1998.6
LL-Null:	-2272.8
LLR p-value:	7.901E-120

Table B.270: Descriptors: Triplet-Unassigned: isSwitch - isUnstruct + Vkabat

Name	**Beta**	**Std Err**	**Z-score**	**P-value**
Intercept	-4.0356	0.118	-34.147	0.0
isUnstruct	3.1972	0.136	23.545	0.0
Vkabat	-0.0961	0.031	-3.064	0.002

Table B.271: Fields: Triplet-Unassigned: isSwitch - isUnstruct + Residue Type

Field	**Value**
Accuracy:	91.36116152450091
Df Residuals:	13776
Df Model:	20
Date:	Thu Apr 04 16:29:04 PDT 2019
Pseudo R-squ.:	0.1259
Log-Likelihood:	-1986.8
LL-Null:	-2272.8
LLR p-value:	2.157E-108

Table B.272: Descriptors: Triplet-Unassigned: isSwitch - isUnstruct + Residue Type

Name	Beta	Std Err	Z-score	P-value
Intercept	-5.1011	0.288	-17.705	0.0
Alanine (A)	1.0788	0.319	3.379	0.001
Arginine (R)	0.4141	0.362	1.143	0.253
Asparagine (N)	1.0656	0.344	3.102	0.002
Aspartic acid (D)	1.1369	0.327	3.477	0.001
Cysteine (C)	1.2305	0.51	2.412	0.016
Glutamine (Q)	0.686	0.326	2.103	0.035
Glutamic acid (E)	0.6814	0.351	1.943	0.052
Glycine (G)	0.9978	0.335	2.979	0.003
Histidine (H)	0.6736	0.431	1.562	0.118
Isoleucine (I)	0.5642	0.368	1.532	0.125
Leucine (L)	0.6908	0.325	2.123	0.034
Lysine (K)	1.0512	0.32	3.285	0.001
Methionine (M)	0.767	0.377	2.032	0.042
Phenylalanine (F)	0.5253	0.429	1.225	0.221
Proline (P)	0.6966	0.351	1.982	0.047
Serine (S)	0.9502	0.32	2.965	0.003
Threonine (T)	0.9561	0.342	2.794	0.005
Tryptophan (W)	0.9329	0.586	1.592	0.111
Tyrosine (Y)	0.4785	0.429	1.116	0.264
isUnstruct	3.1806	0.141	22.5	0.0

Table B.273: Fields: Triplet-Unassigned: isSwitch - Vkabat + Residue Type

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13776
Df Model:	20
Date:	Thu Apr 04 16:29:04 PDT 2019
Pseudo R-squ.:	0.02386
Log-Likelihood:	-2218.6
LL-Null:	-2272.8
LLR p-value:	3.780E-14

Table B.274: Descriptors: Triplet-Unassigned: isSwitch - Vkabat + Residue Type

Name	Beta	Std Err	Z-score	P-value
Intercept	-3.8203	0.293	-13.022	0.0
Alanine (A)	1.2217	0.315	3.885	0.0
Arginine (R)	0.7239	0.357	2.03	0.042
Asparagine (N)	1.2429	0.337	3.692	0.0
Aspartic acid (D)	1.3129	0.322	4.083	0.0
Cysteine (C)	0.9704	0.501	1.935	0.053
Glutamine (Q)	1.0573	0.321	3.293	0.001
Glutamic acid (E)	1.1051	0.344	3.21	0.001
Glycine (G)	0.9615	0.33	2.912	0.004
Histidine (H)	0.6789	0.426	1.595	0.111
Isoleucine (I)	0.5165	0.363	1.421	0.155
Leucine (L)	0.6631	0.321	2.063	0.039
Lysine (K)	1.4355	0.314	4.57	0.0
Methionine (M)	1.491	0.367	4.068	0.0
Phenylalanine (F)	0.2158	0.424	0.509	0.611
Proline (P)	1.1534	0.345	3.342	0.001
Serine (S)	1.5066	0.314	4.796	0.0
Threonine (T)	1.2059	0.336	3.586	0.0
Tryptophan (W)	0.5372	0.578	0.929	0.353
Tyrosine (Y)	0.1505	0.424	0.355	0.723
Vkabat	-0.1366	0.031	-4.399	0.0

Table B.275: Fields: Triplet-Unassigned: isSwitch - E6 + isUnstruct + Vkabat

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13793
Df Model:	3
Date:	Thu Apr 04 16:29:04 PDT 2019
Pseudo R-squ.:	0.1328
Log-Likelihood:	-1971.1
LL-Null:	-2272.8
LLR p-value:	1.760E-130

Table B.276: Descriptors: Triplet-Unassigned: isSwitch - E6 + isUnstruct + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-4.4207	0.132	-33.368	0.0
E6	0.689	0.091	7.553	0.0
isUnstruct	3.0696	0.138	22.18	0.0
Vkabat	-0.0921	0.031	-2.924	0.003

Table B.277: Fields: Triplet-Unassigned: isSwitch - E6 + Residue Type + Vkabat

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13775
Df Model:	21
Date:	Thu Apr 04 16:29:05 PDT 2019
Pseudo R-squ.:	0.04412
Log-Likelihood:	-2172.6
LL-Null:	-2272.8
LLR p-value:	2.833E-31

Table B.278: Descriptors: Triplet-Unassigned: isSwitch - E6 + Residue Type + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-4.241	0.299	-14.205	0.0
Alanine (A)	1.0759	0.316	3.409	0.001
Arginine (R)	0.5442	0.358	1.52	0.128
Asparagine (N)	1.0896	0.338	3.223	0.001
Aspartic acid (D)	1.1065	0.323	3.423	0.001
Cysteine (C)	0.8772	0.503	1.744	0.081
Glutamine (Q)	0.8936	0.322	2.773	0.006
Glutamic acid (E)	0.9533	0.345	2.76	0.006
Glycine (G)	0.8157	0.332	2.46	0.014
Histidine (H)	0.545	0.427	1.277	0.202
Isoleucine (I)	0.5255	0.364	1.444	0.149
Leucine (L)	0.6826	0.322	2.121	0.034
Lysine (K)	1.299	0.315	4.121	0.0
Methionine (M)	1.4913	0.367	4.058	0.0
Phenylalanine (F)	0.2166	0.425	0.51	0.61
Proline (P)	0.9672	0.347	2.787	0.005
Serine (S)	1.3226	0.315	4.192	0.0
Threonine (T)	1.0713	0.337	3.174	0.002
Tryptophan (W)	0.5879	0.579	1.015	0.31
Tyrosine (Y)	0.1785	0.425	0.42	0.674
E6	0.867	0.088	9.833	0.0
Vkabat	-0.1326	0.031	-4.262	0.0

Table B.279: Fields: Triplet-Unassigned: isSwitch - E6 + Residue Type + isUnstruct

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13775
Df Model:	21
Date:	Thu Apr 04 16:29:05 PDT 2019
Pseudo R-squ.:	0.137
Log-Likelihood:	-1961.4
LL-Null:	-2272.8
LLR p-value:	2.430E-118

Table B.280: Descriptors: Triplet-Unassigned: isSwitch - E6 + Residue Type + isUnstruct

Name	Beta	Std Err	Z-score	P-value
Intercept	-5.4106	0.293	-18.457	0.0
Alanine (A)	0.9833	0.32	3.068	0.002
Arginine (R)	0.2957	0.364	0.813	0.416
Asparagine (N)	0.9664	0.345	2.802	0.005
Aspartic acid (D)	1.0171	0.328	3.099	0.002
Cysteine (C)	1.1466	0.514	2.232	0.026
Glutamine (Q)	0.6101	0.327	1.865	0.062
Glutamic acid (E)	0.634	0.351	1.804	0.071
Glycine (G)	0.8927	0.336	2.653	0.008
Histidine (H)	0.5497	0.434	1.267	0.205
Isoleucine (I)	0.5727	0.369	1.552	0.121
Leucine (L)	0.6992	0.326	2.143	0.032
Lysine (K)	1.0002	0.321	3.119	0.002
Methionine (M)	0.8382	0.378	2.22	0.026
Phenylalanine (F)	0.5295	0.43	1.233	0.218
Proline (P)	0.594	0.353	1.684	0.092
Serine (S)	0.8358	0.322	2.597	0.009
Threonine (T)	0.8969	0.343	2.614	0.009
Tryptophan (W)	0.9726	0.587	1.657	0.098
Tyrosine (Y)	0.5112	0.429	1.191	0.234
E6	0.6703	0.093	7.241	0.0
isUnstruct	3.0739	0.143	21.482	0.0

Table B.281: Fields: Triplet-Unassigned: isSwitch - E20 + isUnstruct + Vkabat

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13793
Df Model:	3
Date:	Thu Apr 04 16:29:05 PDT 2019
Pseudo R-squ.:	0.1355
Log-Likelihood:	-1964.9
LL-Null:	-2272.8
LLR p-value:	3.493E-133

Table B.282: Descriptors: Triplet-Unassigned: isSwitch - E20 + isUnstruct + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-4.5001	0.134	-33.467	0.0
E20	0.5144	0.062	8.353	0.0
isUnstruct	3.0997	0.138	22.425	0.0
Vkabat	-0.1026	0.032	-3.25	0.001

Table B.283: Fields: Triplet-Unassigned: isSwitch - E20 + Residue Type + Vkabat

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13775
Df Model:	21
Date:	Thu Apr 04 16:29:05 PDT 2019
Pseudo R-squ.:	0.04596
Log-Likelihood:	-2168.4
LL-Null:	-2272.8
LLR p-value:	6.275E-33

Table B.284: Descriptors: Triplet-Unassigned: isSwitch - E20 + Residue Type + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-4.4012	0.301	-14.631	0.0
Alanine (A)	1.1816	0.315	3.749	0.0
Arginine (R)	0.6509	0.358	1.82	0.069
Asparagine (N)	1.1979	0.338	3.548	0.0
Aspartic acid (D)	1.2143	0.323	3.763	0.0
Cysteine (C)	0.9549	0.503	1.898	0.058
Glutamine (Q)	1.0095	0.322	3.137	0.002
Glutamic acid (E)	1.0909	0.345	3.161	0.002
Glycine (G)	0.9478	0.331	2.863	0.004
Histidine (H)	0.6511	0.426	1.527	0.127
Isoleucine (I)	0.5385	0.364	1.479	0.139
Leucine (L)	0.7433	0.322	2.308	0.021
Lysine (K)	1.4091	0.315	4.474	0.0
Methionine (M)	1.511	0.368	4.109	0.0
Phenylalanine (F)	0.3012	0.425	0.709	0.478
Proline (P)	1.1159	0.346	3.222	0.001
Serine (S)	1.4322	0.315	4.547	0.0
Threonine (T)	1.1554	0.337	3.426	0.001
Tryptophan (W)	0.7221	0.58	1.246	0.213
Tyrosine (Y)	0.256	0.425	0.603	0.547
E20	0.6121	0.06	10.259	0.0
Vkabat	-0.1403	0.031	-4.5	0.0

Table B.285: Fields: Triplet-Unassigned: isSwitch - E20 + Residue Type + isUnstruct

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13775
Df Model:	21
Date:	Thu Apr 04 16:29:05 PDT 2019
Pseudo R-squ.:	0.1398
Log-Likelihood:	-1955.1
LL-Null:	-2272.8
LLR p-value:	5.665E-121

Table B.286: Descriptors: Triplet-Unassigned: isSwitch - E20 + Residue Type + isUnstruct

Name	Beta	Std Err	Z-score	P-value
Intercept	-5.5736	0.297	-18.79	0.0
Alanine (A)	1.0501	0.321	3.276	0.001
Arginine (R)	0.3616	0.363	0.995	0.32
Asparagine (N)	1.0288	0.345	2.982	0.003
Aspartic acid (D)	1.0825	0.328	3.299	0.001
Cysteine (C)	1.1996	0.514	2.335	0.02
Glutamine (Q)	0.6847	0.327	2.093	0.036
Glutamic acid (E)	0.7253	0.352	2.063	0.039
Glycine (G)	0.9887	0.336	2.941	0.003
Histidine (H)	0.6169	0.434	1.421	0.155
Isoleucine (I)	0.5708	0.369	1.546	0.122
Leucine (L)	0.7419	0.327	2.272	0.023
Lysine (K)	1.071	0.321	3.339	0.001
Methionine (M)	0.8499	0.378	2.25	0.024
Phenylalanine (F)	0.5911	0.43	1.375	0.169
Proline (P)	0.7014	0.353	1.99	0.047
Serine (S)	0.9053	0.322	2.814	0.005
Threonine (T)	0.9392	0.344	2.734	0.006
Tryptophan (W)	1.081	0.587	1.841	0.066
Tyrosine (Y)	0.575	0.43	1.339	0.181
E20	0.4998	0.062	8.084	0.0
isUnstruct	3.0977	0.143	21.631	0.0

Table B.287: Fields: Triplet-Unassigned: isSwitch - Residue Type + isUnstruct + Vkabat

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13775
Df Model:	21
Date:	Thu Apr 04 16:29:06 PDT 2019
Pseudo R-squ.:	0.1273
Log-Likelihood:	-1983.4
LL-Null:	-2272.8
LLR p-value:	4.409E-109

Table B.288: Descriptors: Triplet-Unassigned: isSwitch - Residue Type + isUnstruct + Vkabat

Name	Beta	Std Err	Z-score	P-value
Intercept	-4.8241	0.306	-15.762	0.0
Alanine (A)	1.0313	0.32	3.226	0.001
Arginine (R)	0.4046	0.362	1.117	0.264
Asparagine (N)	1.0052	0.344	2.918	0.004
Aspartic acid (D)	1.0833	0.328	3.307	0.001
Cysteine (C)	1.1973	0.511	2.345	0.019
Glutamine (Q)	0.6407	0.327	1.961	0.05
Glutamic acid (E)	0.6297	0.351	1.792	0.073
Glycine (G)	0.9198	0.336	2.736	0.006
Histidine (H)	0.6455	0.432	1.496	0.135
Isoleucine (I)	0.5711	0.368	1.552	0.121
Leucine (L)	0.6571	0.326	2.018	0.044
Lysine (K)	1.0132	0.32	3.164	0.002
Methionine (M)	0.7414	0.378	1.963	0.05
Phenylalanine (F)	0.5096	0.429	1.189	0.235
Proline (P)	0.6102	0.353	1.729	0.084
Serine (S)	0.9129	0.321	2.845	0.004
Threonine (T)	0.9426	0.342	2.754	0.006
Tryptophan (W)	0.9216	0.586	1.571	0.116
Tyrosine (Y)	0.4592	0.429	1.071	0.284
isUnstruct	3.1495	0.142	22.177	0.0
Vkabat	-0.0822	0.032	-2.565	0.01

Table B.289: Fields: Triplet-Unassigned: isSwitch - E6 + Residue Type + isUnstruct + Vkabat

Field	Value
Accuracy:	91.36116152450091
Df Residuals:	13774
Df Model:	22
Date:	Thu Apr 04 16:29:06 PDT 2019
Pseudo R-squ.:	0.1385
Log-Likelihood:	-1958.1
LL-Null:	-2272.8
LLR p-value:	5.623E-119

Table B.290: Descriptors: Triplet-Unassigned: isSwitch - E6 + Residue Type + isUnstruct + Vkabat

Name	**Beta**	**Std Err**	**Z-score**	**P-value**
Intercept	-5.1338	0.311	-16.491	0.0
Alanine (A)	0.9344	0.321	2.911	0.004
Arginine (R)	0.2803	0.364	0.77	0.441
Asparagine (N)	0.9055	0.346	2.618	0.009
Aspartic acid (D)	0.9589	0.329	2.915	0.004
Cysteine (C)	1.1126	0.514	2.164	0.03
Glutamine (Q)	0.5637	0.328	1.721	0.085
Glutamic acid (E)	0.5805	0.352	1.649	0.099
Glycine (G)	0.8095	0.338	2.395	0.017
Histidine (H)	0.5183	0.434	1.193	0.233
Isoleucine (I)	0.5774	0.369	1.565	0.118
Leucine (L)	0.6655	0.326	2.039	0.041
Lysine (K)	0.9595	0.321	2.989	0.003
Methionine (M)	0.8089	0.378	2.142	0.032
Phenylalanine (F)	0.5143	0.429	1.198	0.231
Proline (P)	0.5045	0.354	1.423	0.155
Serine (S)	0.7947	0.322	2.465	0.014
Threonine (T)	0.877	0.343	2.554	0.011
Tryptophan (W)	0.9561	0.587	1.628	0.104
Tyrosine (Y)	0.489	0.429	1.139	0.255
E6	0.6697	0.093	7.224	0.0
isUnstruct	3.0436	0.144	21.175	0.0
Vkabat	-0.0812	0.032	-2.522	0.012

Table B.291: Fields: Triplet-Unassigned: isSwitch - E20 + Residue Type + isUnstruct + Vkabat

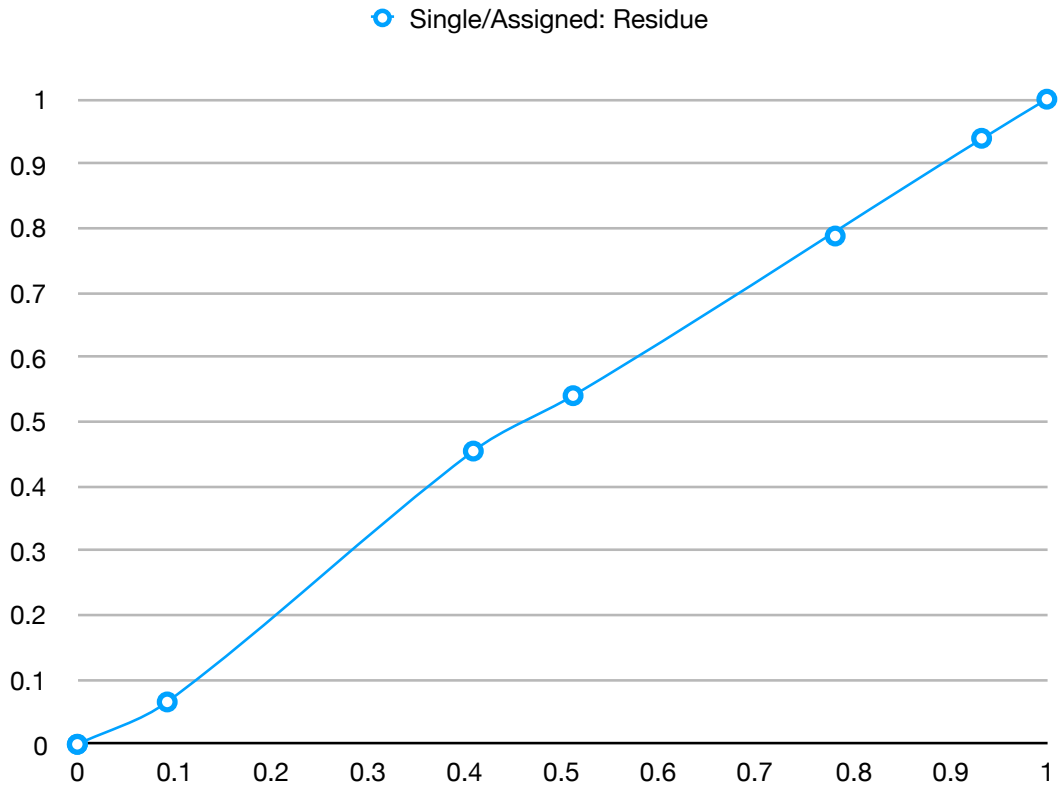
Field	**Value**
Accuracy:	91.36116152450091
Df Residuals:	13774
Df Model:	22
Date:	Thu Apr 04 16:29:06 PDT 2019
Pseudo R-squ.:	0.1415
Log-Likelihood:	-1951.2
LL-Null:	-2272.8
LLR p-value:	6.739E-122

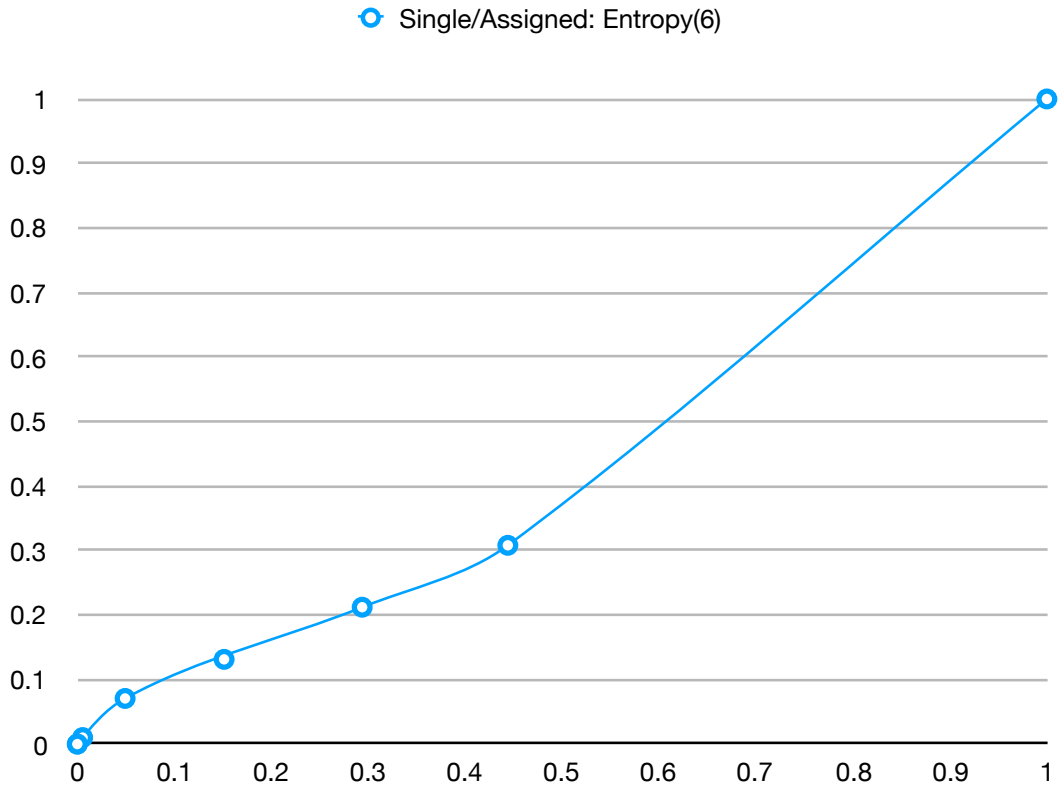
Table B.292: Descriptors: Triplet-Unassigned: isSwitch - E20 + Residue Type + isUnstruct + Vkabat

Name	**Beta**	**Std Err**	**Z-score**	**P-value**
Intercept	-5.2768	0.313	-16.833	0.0
Alanine (A)	0.9975	0.321	3.109	0.002
Arginine (R)	0.3449	0.364	0.949	0.343
Asparagine (N)	0.9631	0.346	2.785	0.005
Aspartic acid (D)	1.0181	0.329	3.097	0.002
Cysteine (C)	1.1631	0.514	2.262	0.024
Glutamine (Q)	0.6341	0.327	1.936	0.053
Glutamic acid (E)	0.6677	0.352	1.896	0.058
Glycine (G)	0.8988	0.338	2.662	0.008
Histidine (H)	0.5829	0.435	1.342	0.18
Isoleucine (I)	0.5763	0.369	1.562	0.118
Leucine (L)	0.7063	0.327	2.162	0.031
Lysine (K)	1.0278	0.321	3.202	0.001
Methionine (M)	0.8188	0.378	2.167	0.03
Phenylalanine (F)	0.5758	0.43	1.34	0.18
Proline (P)	0.6028	0.354	1.702	0.089
Serine (S)	0.8614	0.322	2.674	0.007
Threonine (T)	0.9182	0.344	2.672	0.008
Tryptophan (W)	1.0653	0.588	1.813	0.07
Tyrosine (Y)	0.551	0.429	1.283	0.199
E20	0.506	0.062	8.156	0.0
isUnstruct	3.0642	0.144	21.301	0.0
Vkabat	-0.0894	0.032	-2.773	0.006

APPENDIX C

ROC Plots

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0.5
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0.6
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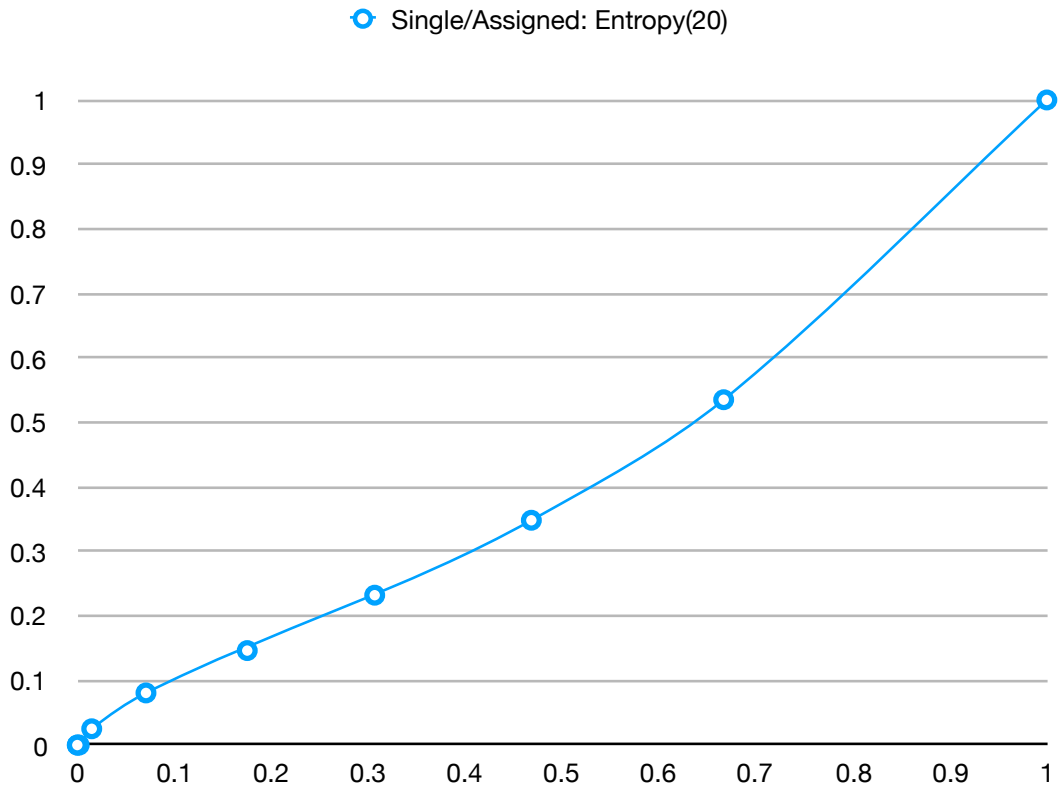
0.8
0.9
1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0.6
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0.8
0.9
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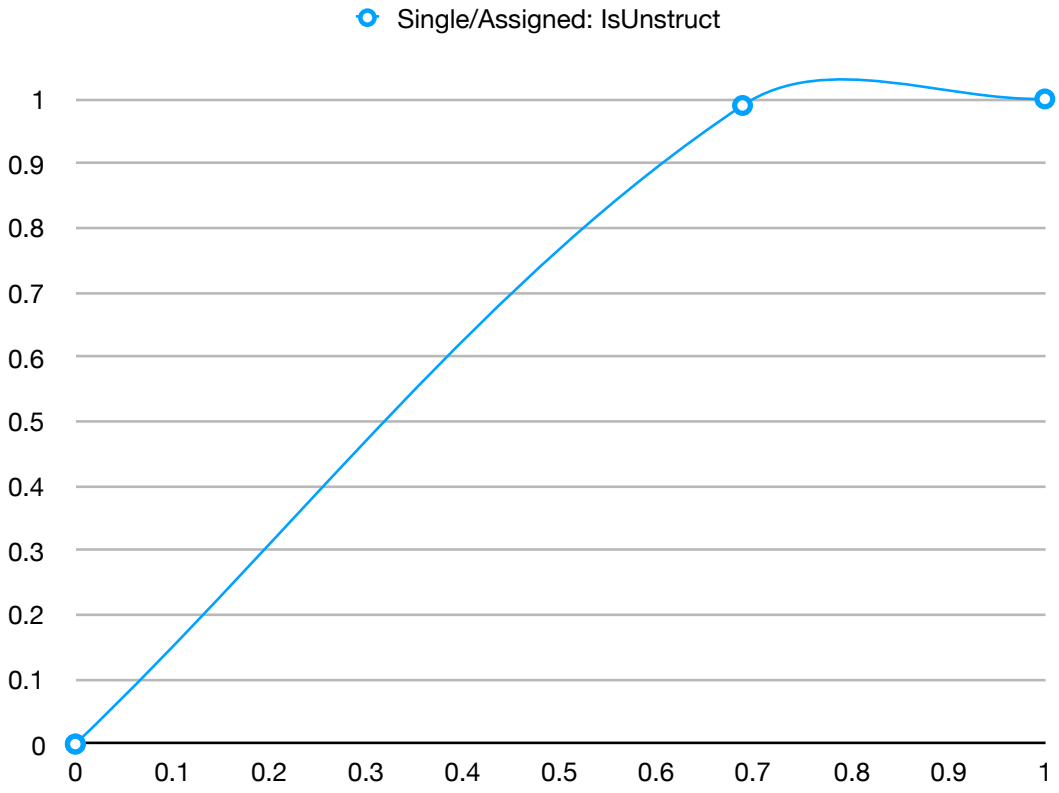
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0.6
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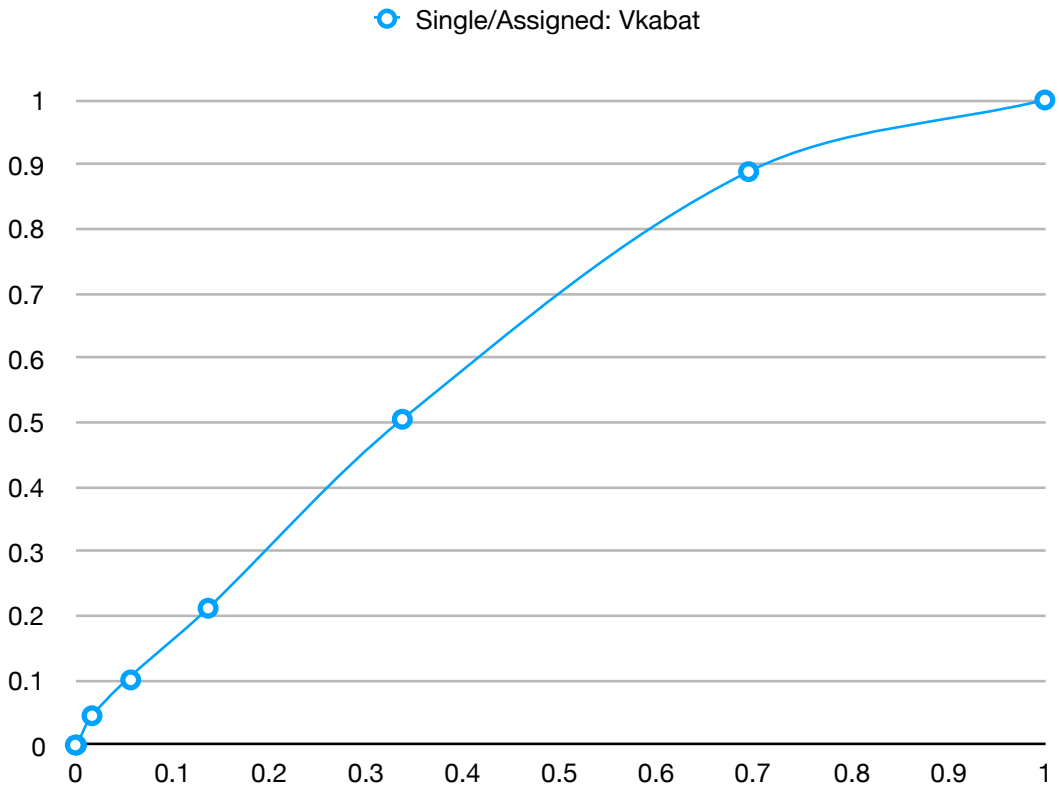
1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0.6
0.5
0.4
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0.2
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0.6
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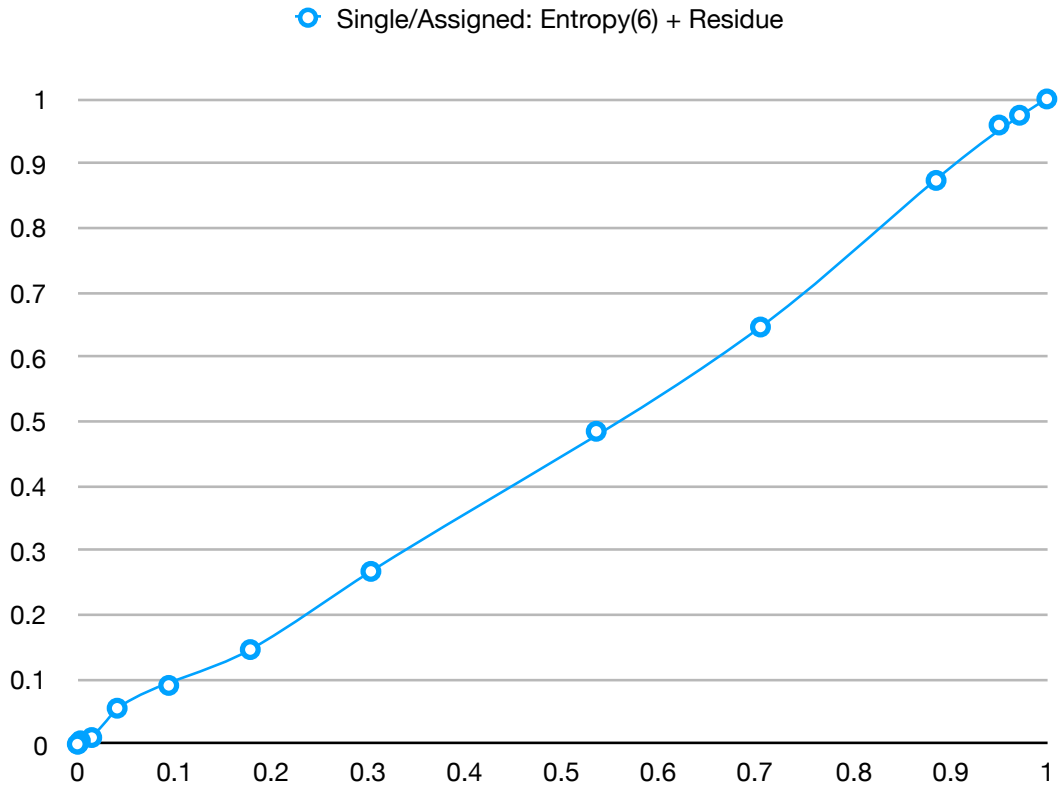
0.8
0.9
1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0.7
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0.5
0.4
0.3
0.2
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0.9
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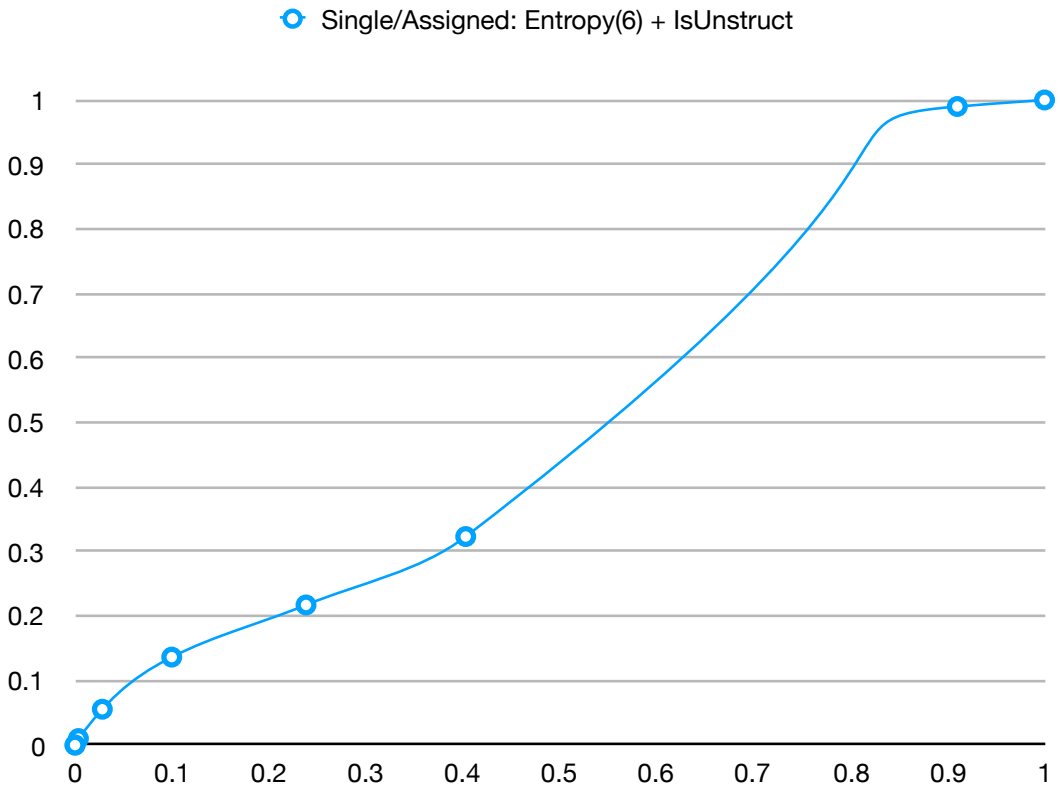
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0.8
0.7
0.6
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0.3
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0.3
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0.6
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0.8
0.9
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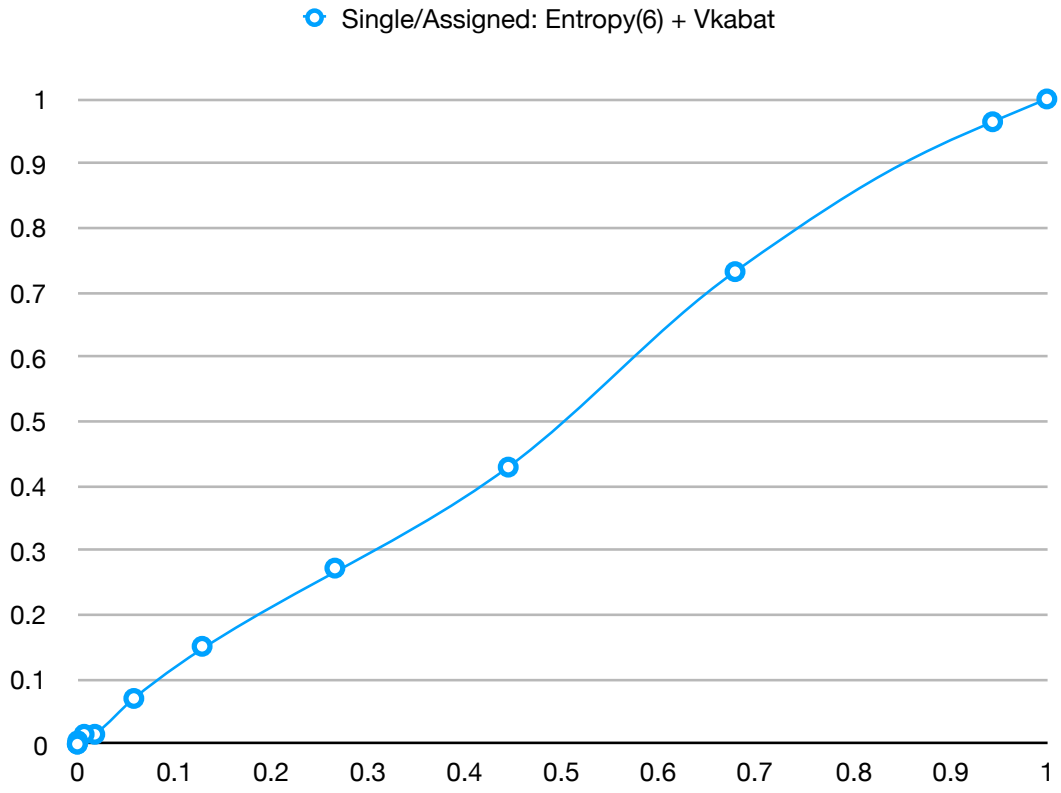
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0.8
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0.4
0.3
0.2
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0.2
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0.6
0.7
0.8
0.9
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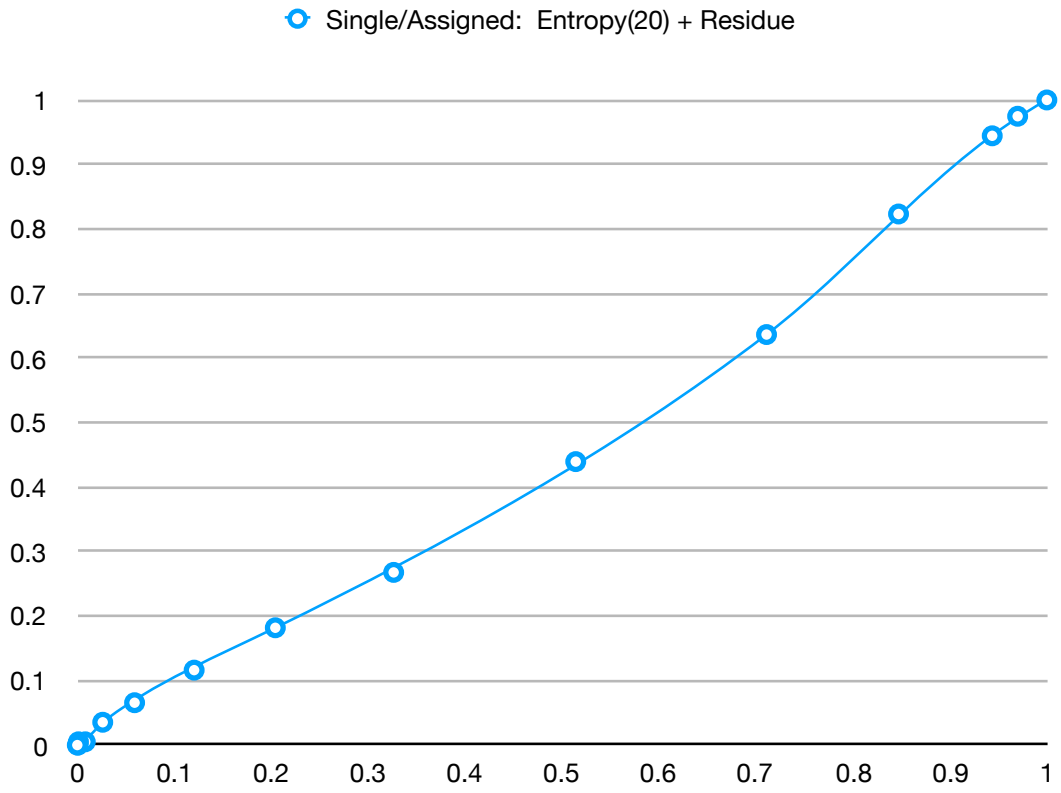
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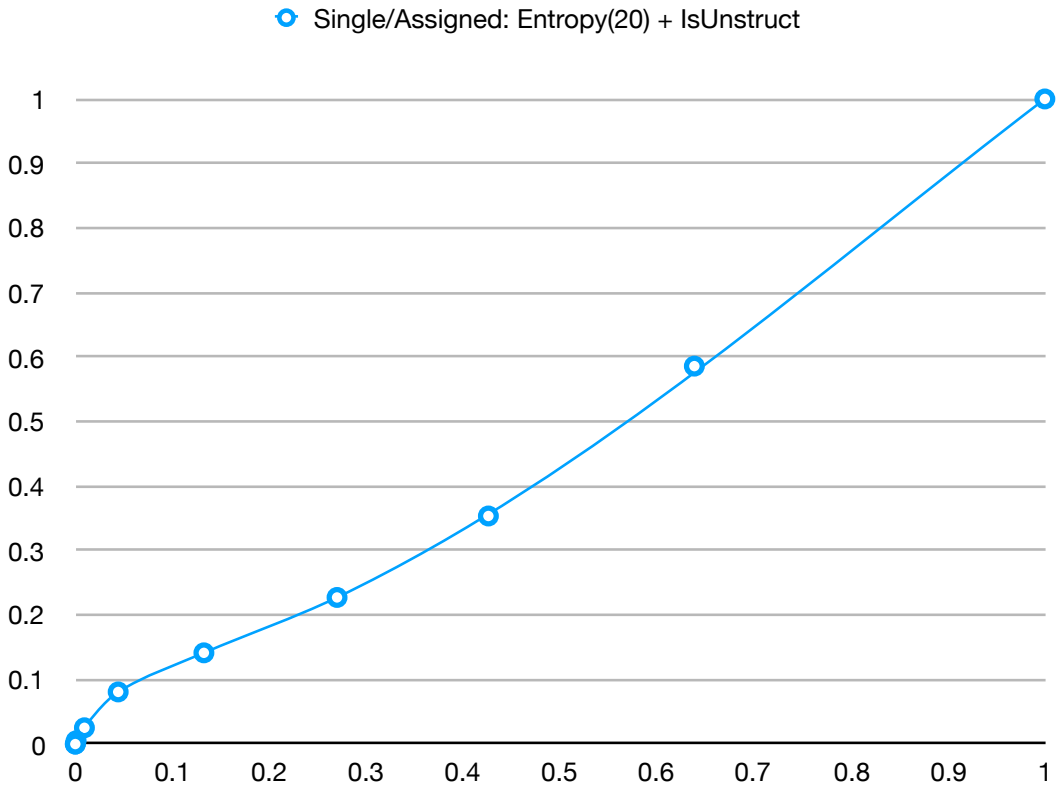
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0.8
0.7
0.6
0.5
0.4
0.3
0.2
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0.1
0.2
0.3
0.4
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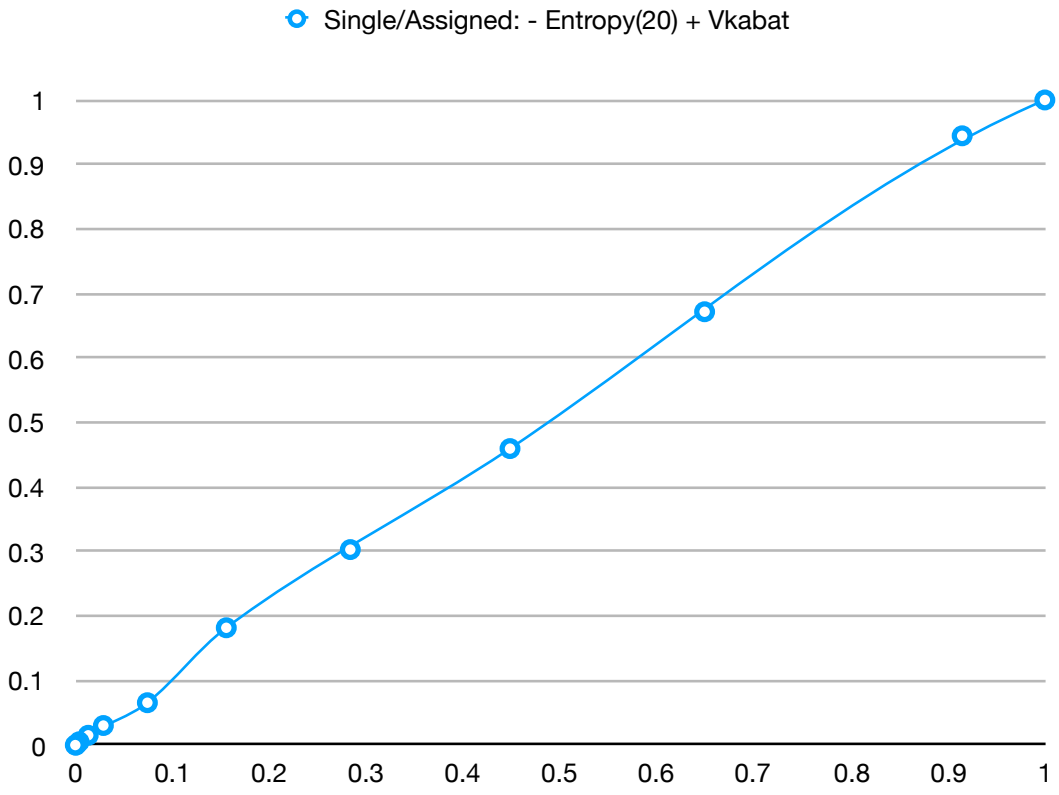
0.6
0.7
0.8
0.9
1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0.4
0.3
0.2
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0.6
0.7
0.8
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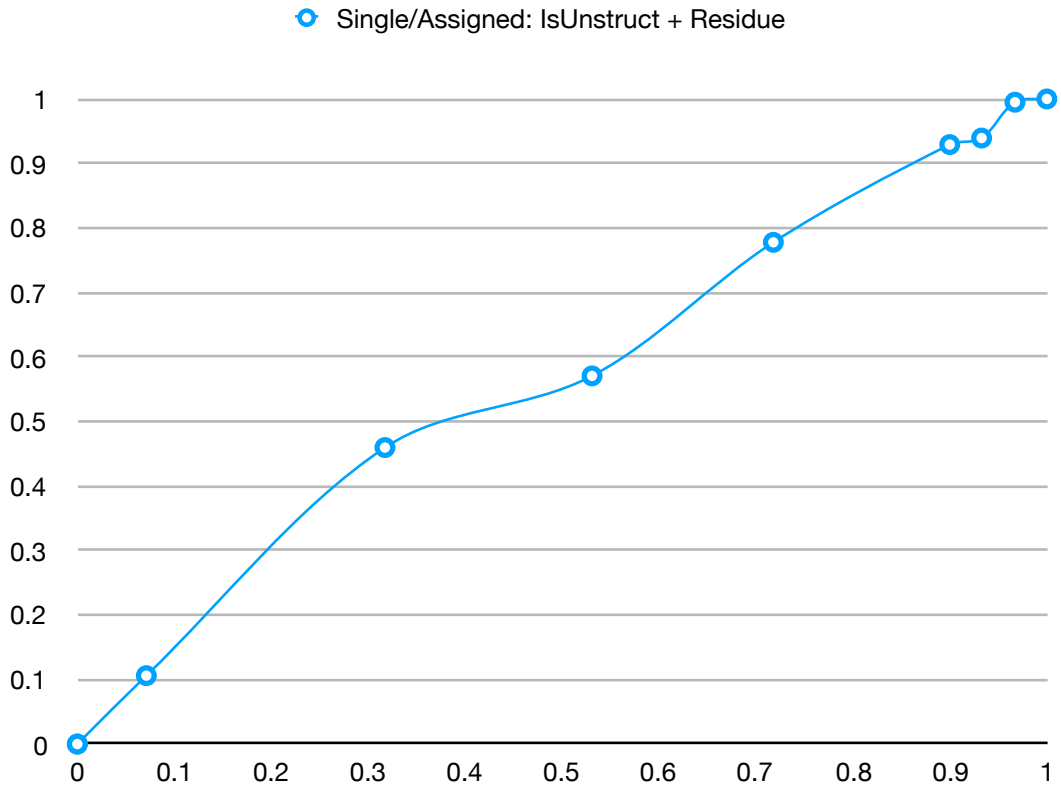
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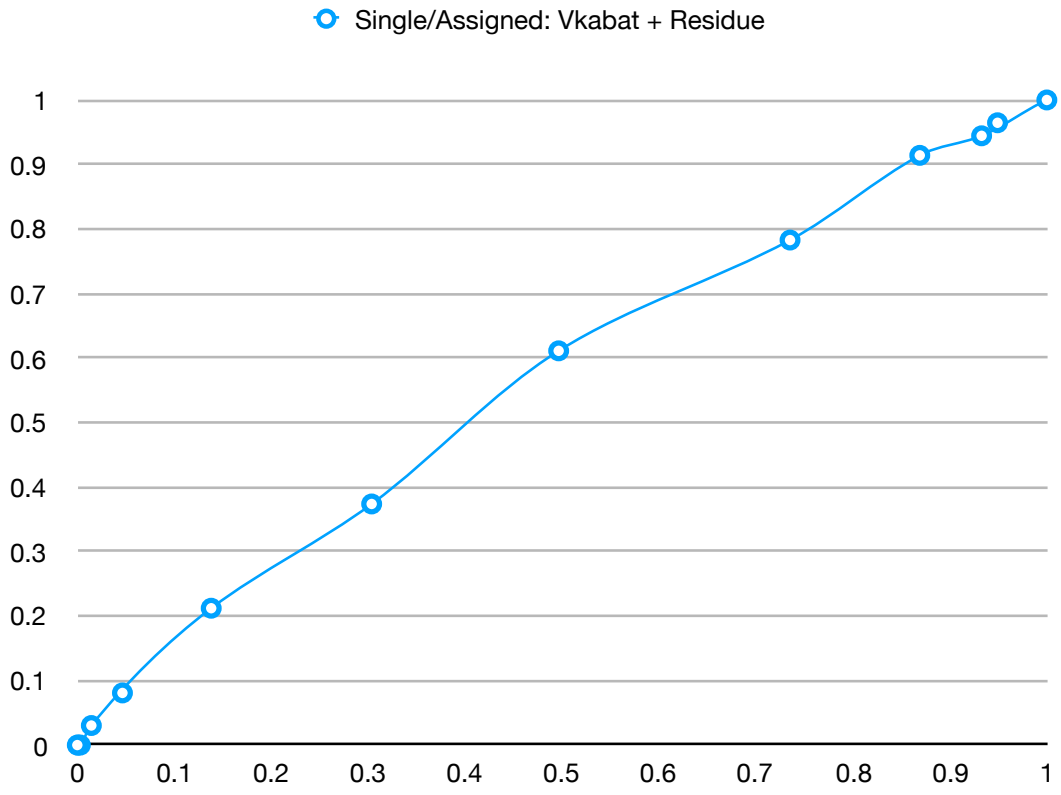
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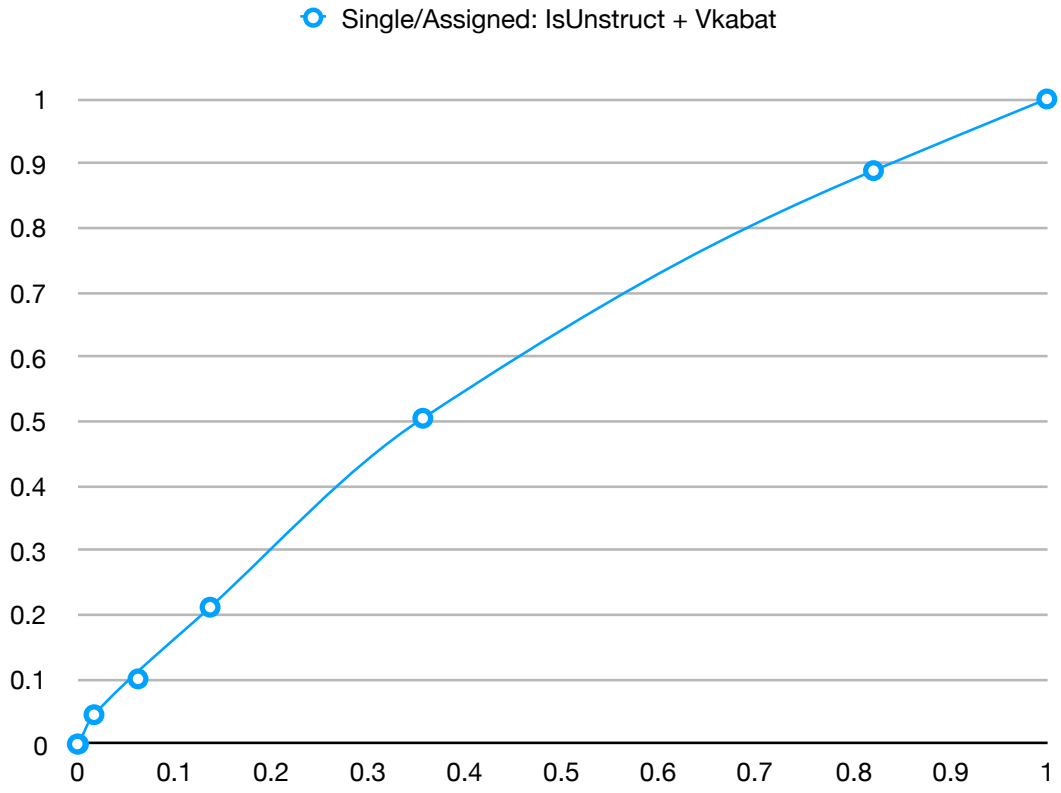
0.8
0.9
1


Single/Assigned: IsUnstruct + Vkabat
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0.9
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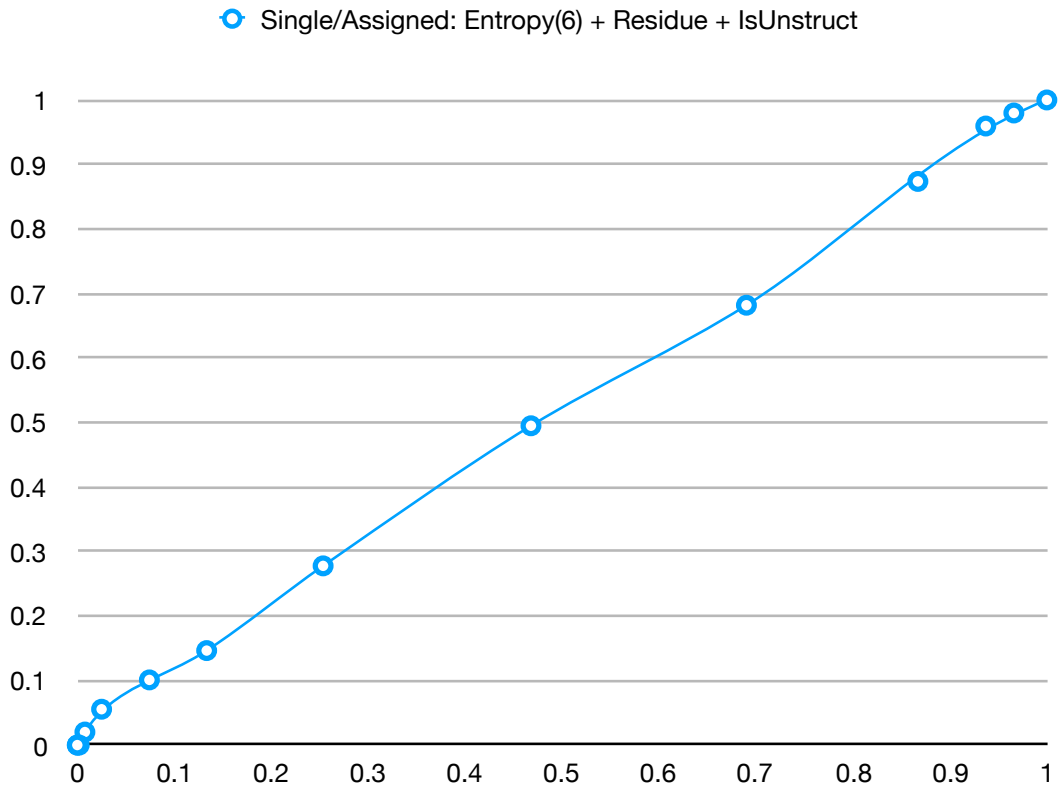
Single/Assigned: Entropy(6) + Residue + IsUnstruct
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0.6
0.5
0.4
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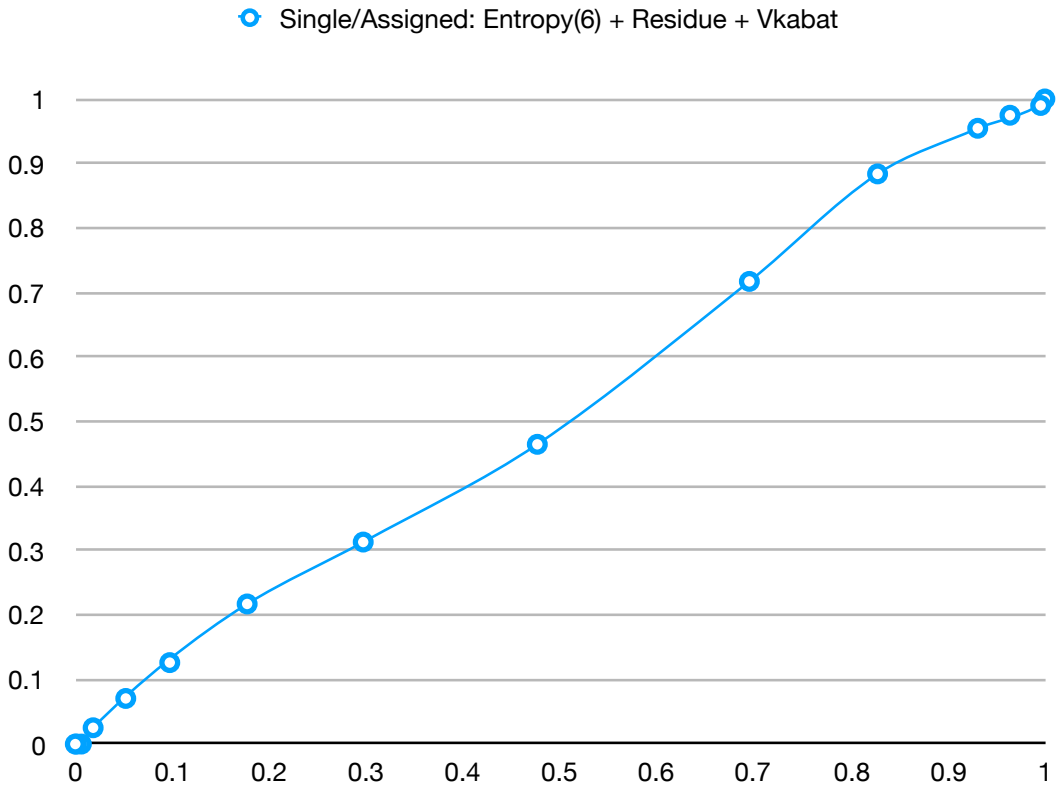
Single/Assigned: Entropy(6) + Residue + Vkabat
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0.7
0.6
0.5
0.4
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0.6
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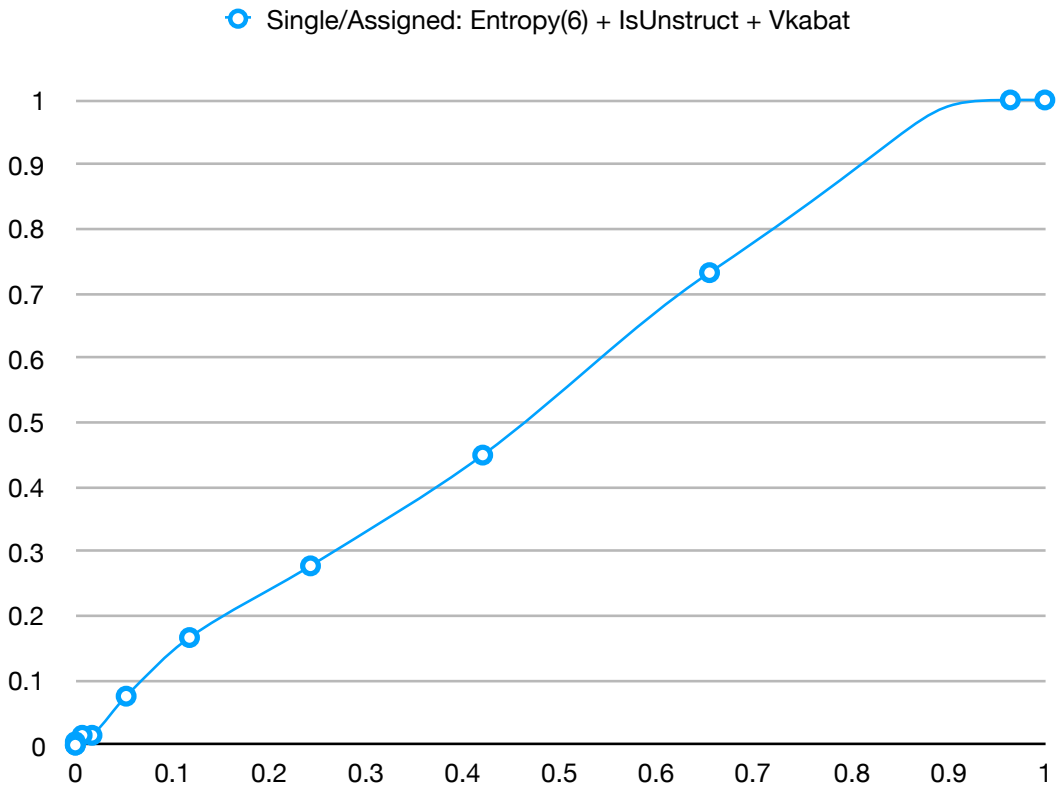
0.8
0.9
1


Single/Assigned: Entropy(6) + IsUnstruct + Vkabat
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0.7
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0.5
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0.2
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0.4
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0.9
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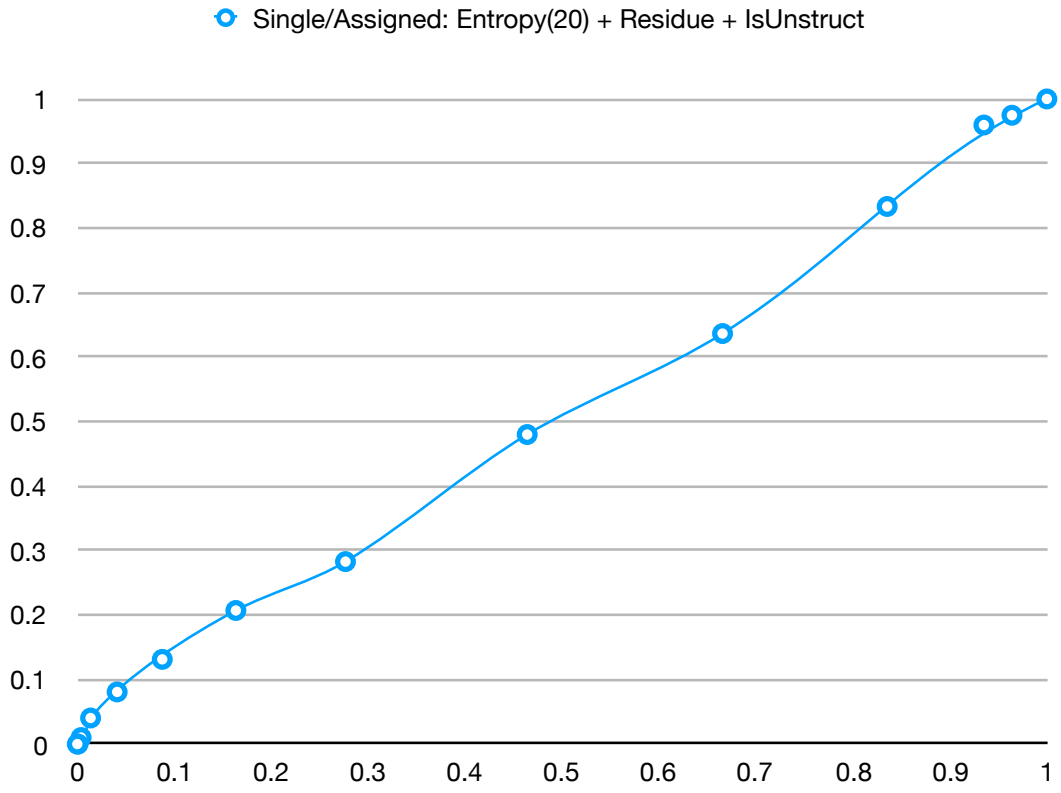
Single/Assigned: Entropy(20) + Residue + IsUnstruct
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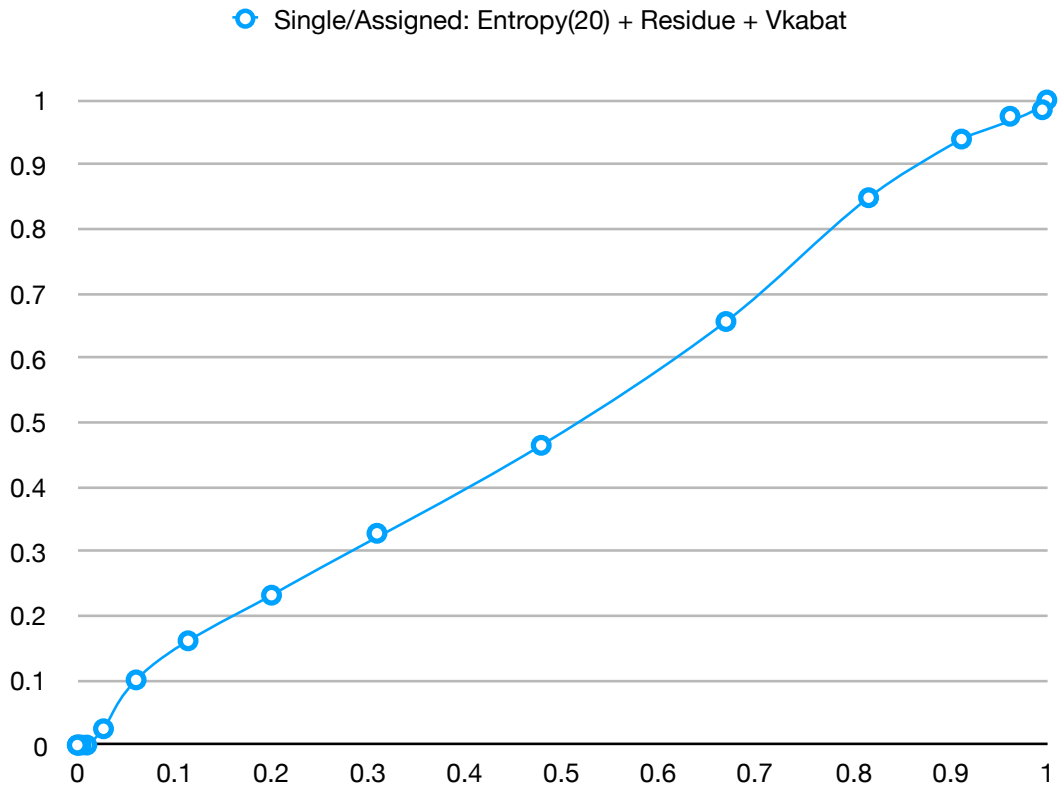
Single/Assigned: Entropy(20) + Residue + Vkabat
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0.8
0.7
0.6
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0.4
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0.2
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0.9
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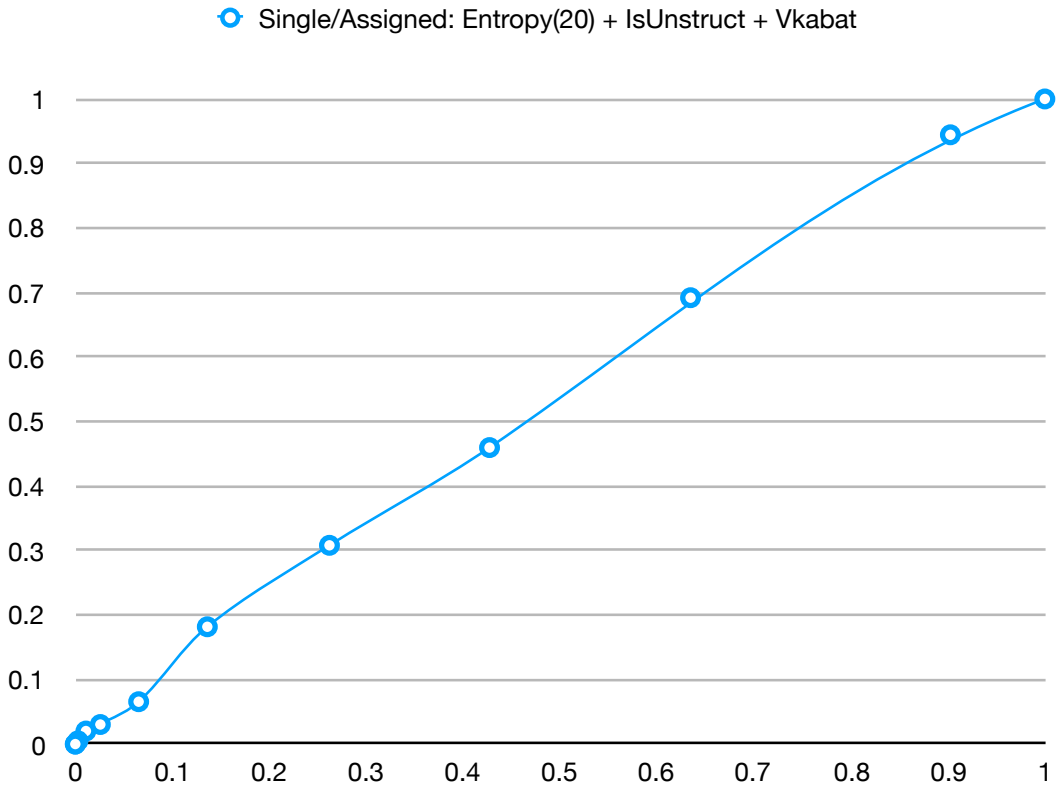
Single/Assigned: Entropy(20) + IsUnstruct + Vkabat
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0.9
0.8
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0.4
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0.2
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0.2
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0.9
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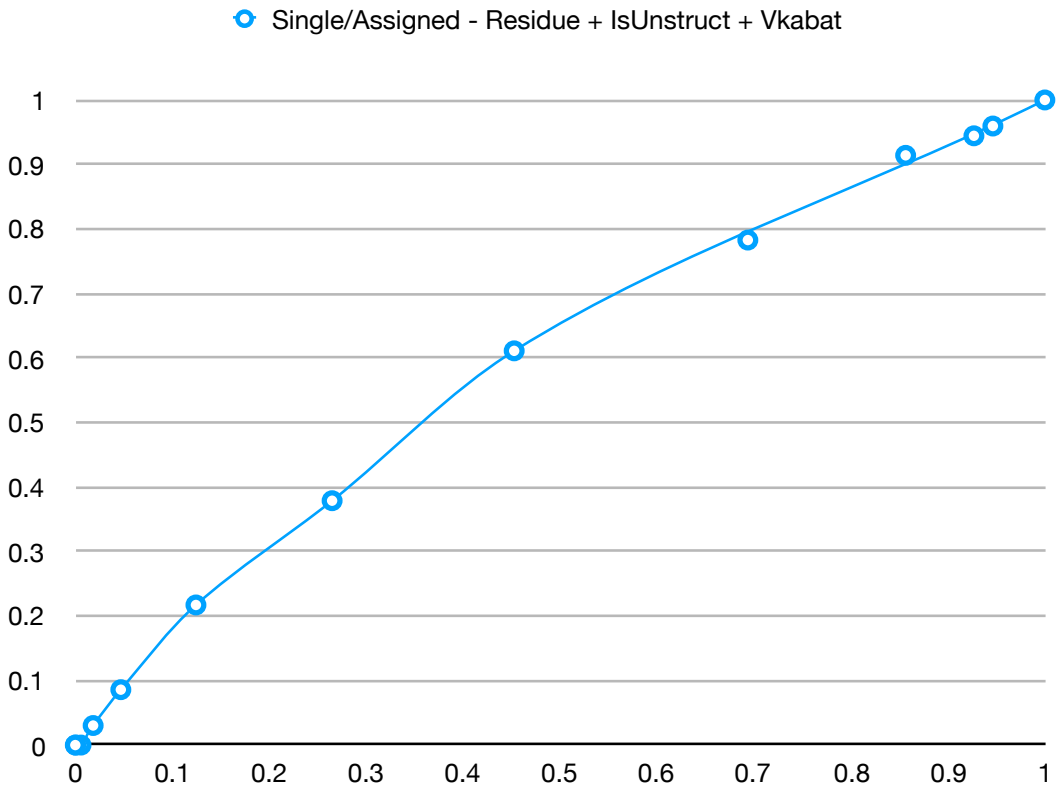
Single/Assigned - Residue + IsUnstruct + Vkabat
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0.7
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0.2
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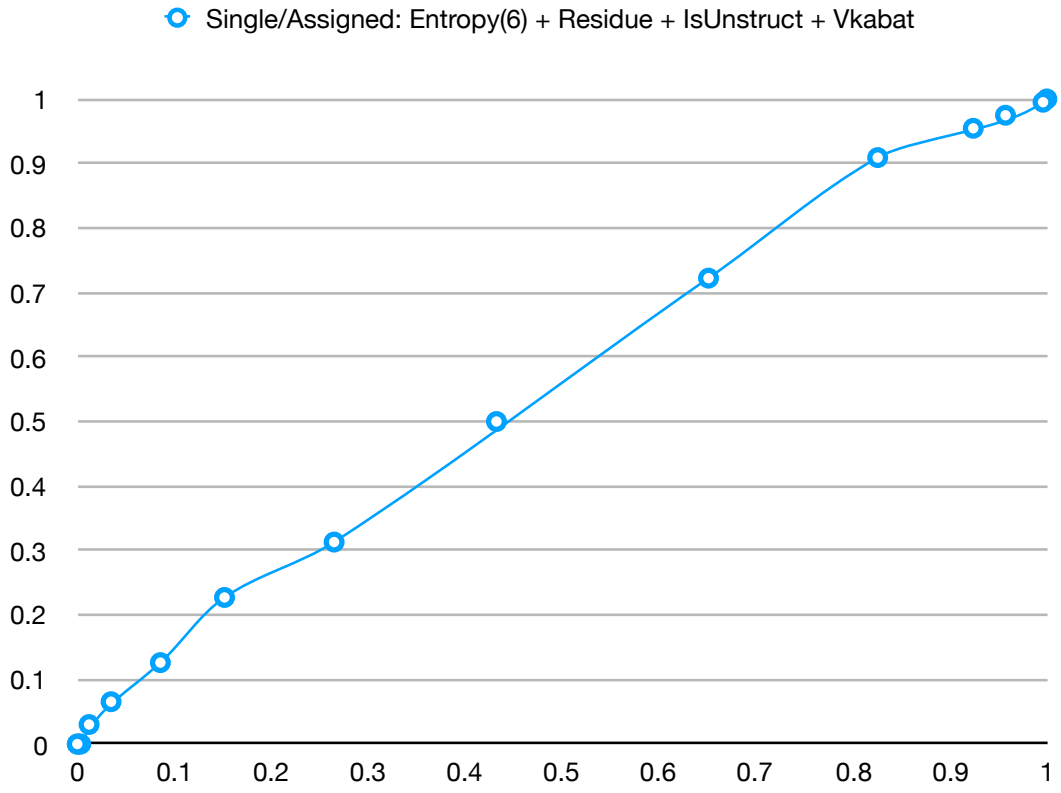
Single/Assigned: Entropy(6) + Residue + IsUnstruct + Vkabat
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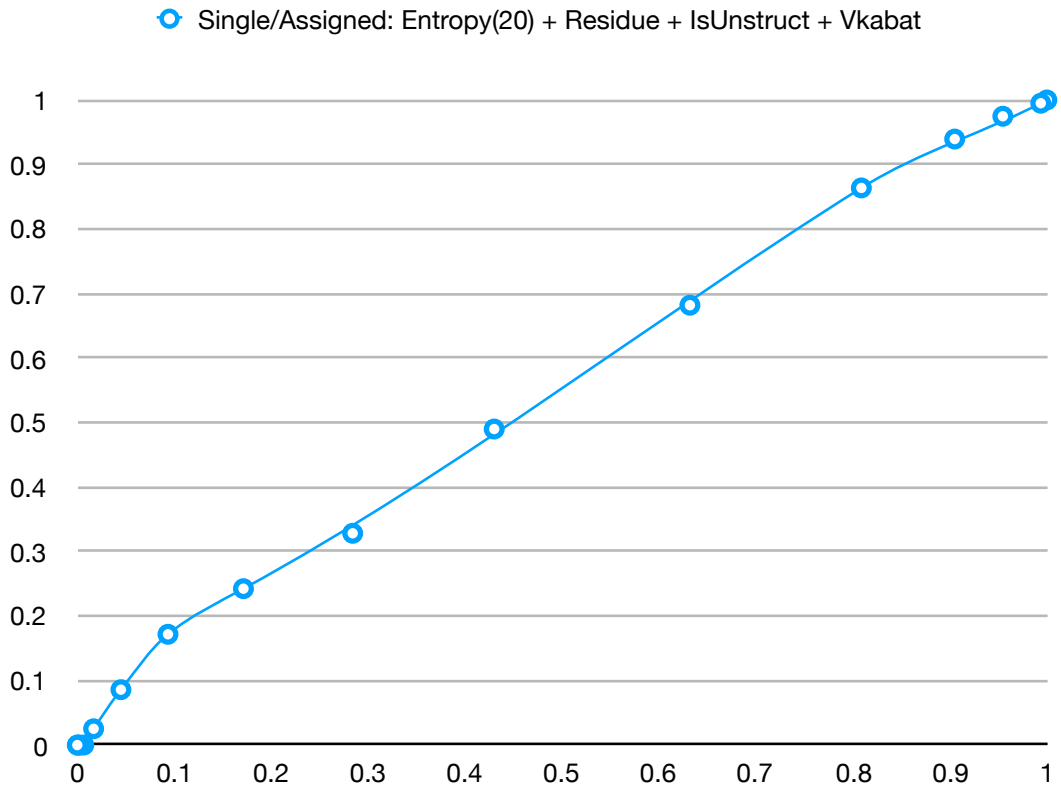
Single/Assigned: Entropy(20) + Residue + IsUnstruct + Vkabat
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0.2
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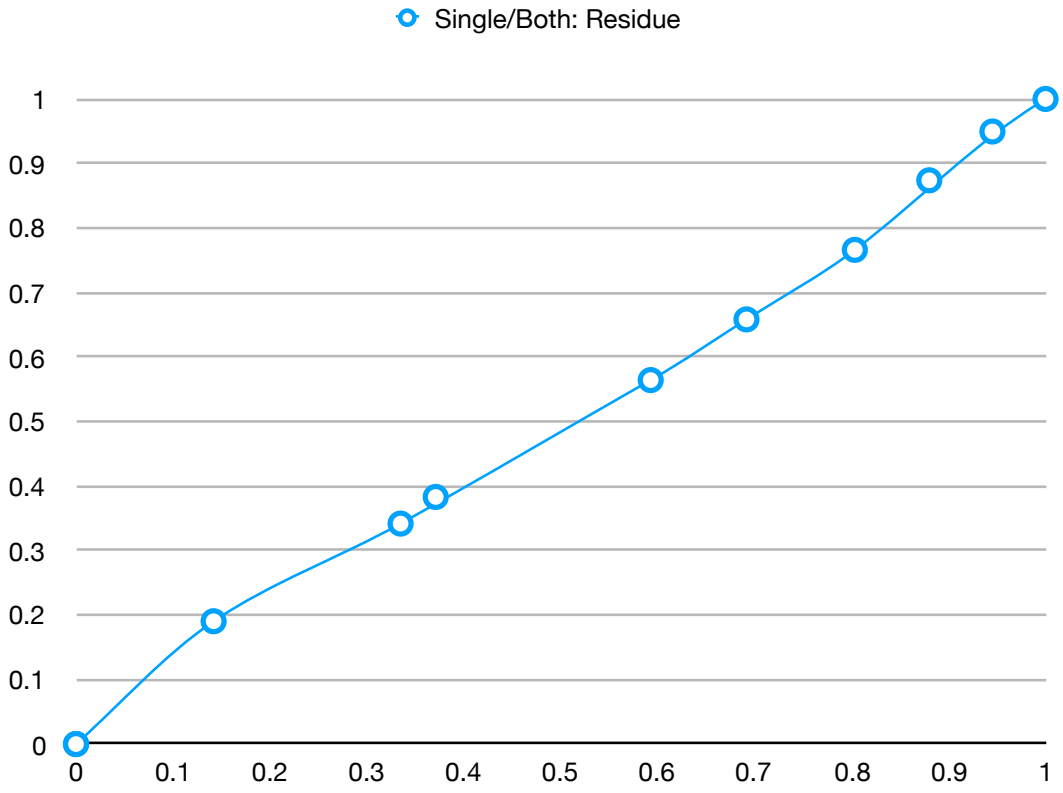
Single/Both: Residue
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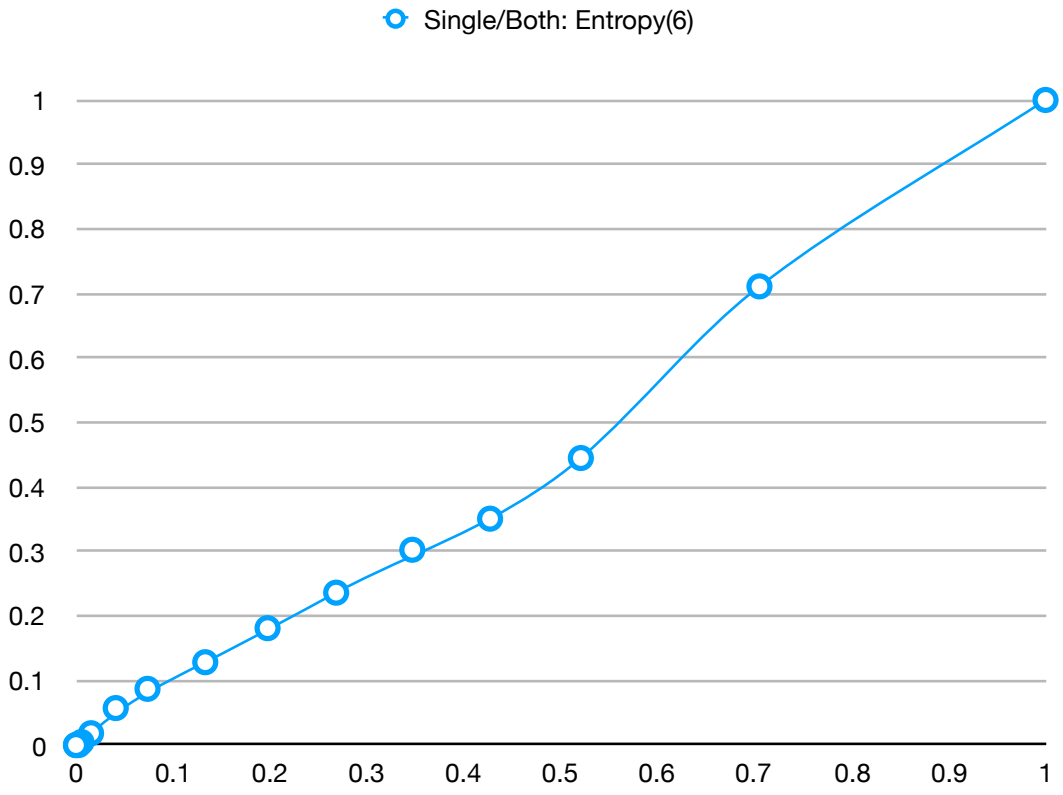
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0.9
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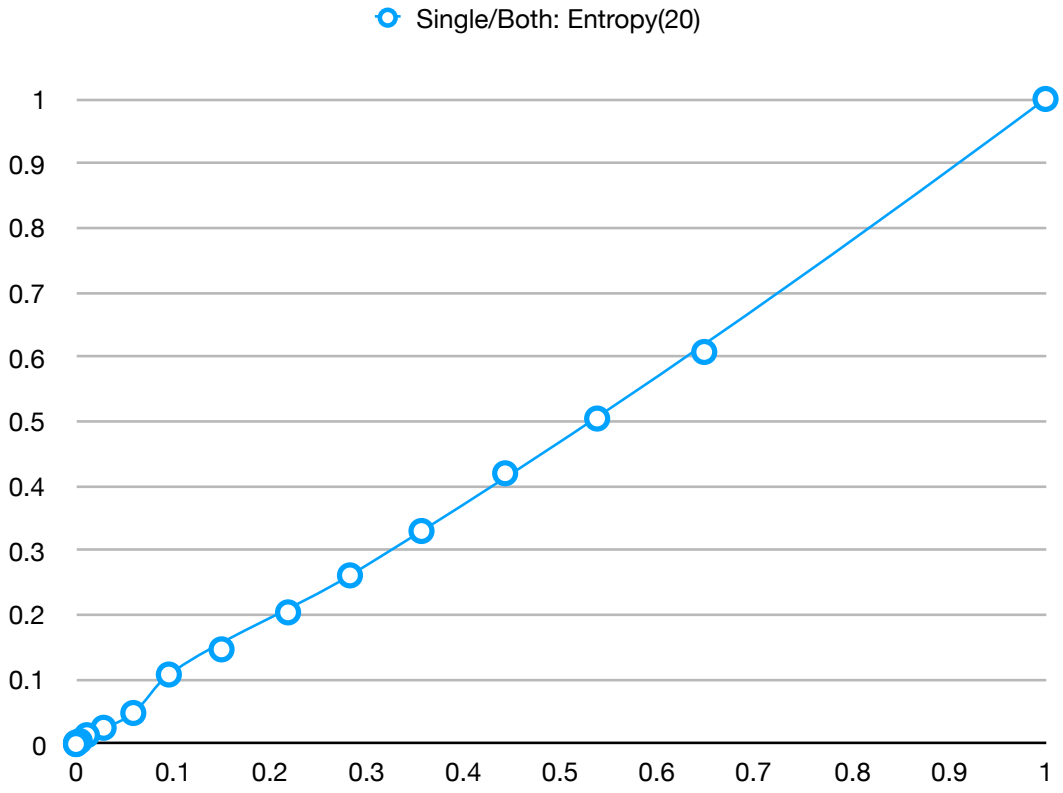
Single/Both: Entropy(20)
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0.2
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0.1
0.2
0.3
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0.8
0.9
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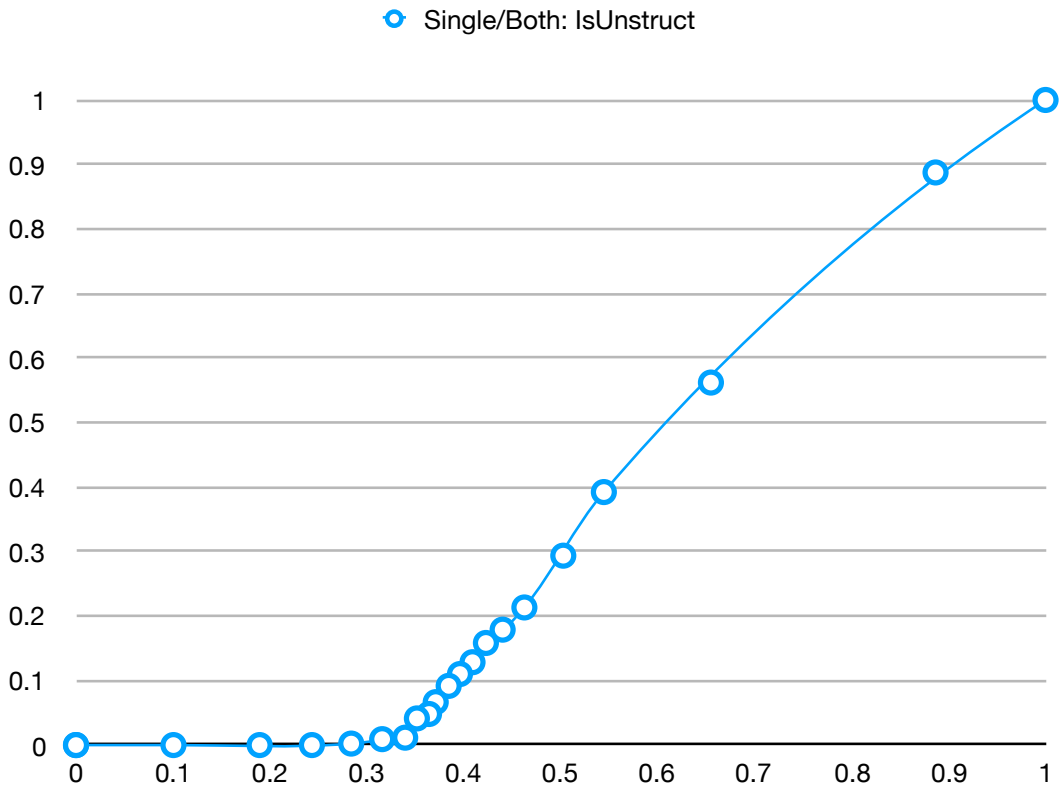
Single/Both: IsUnstruct
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0.4
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0.3
0.4
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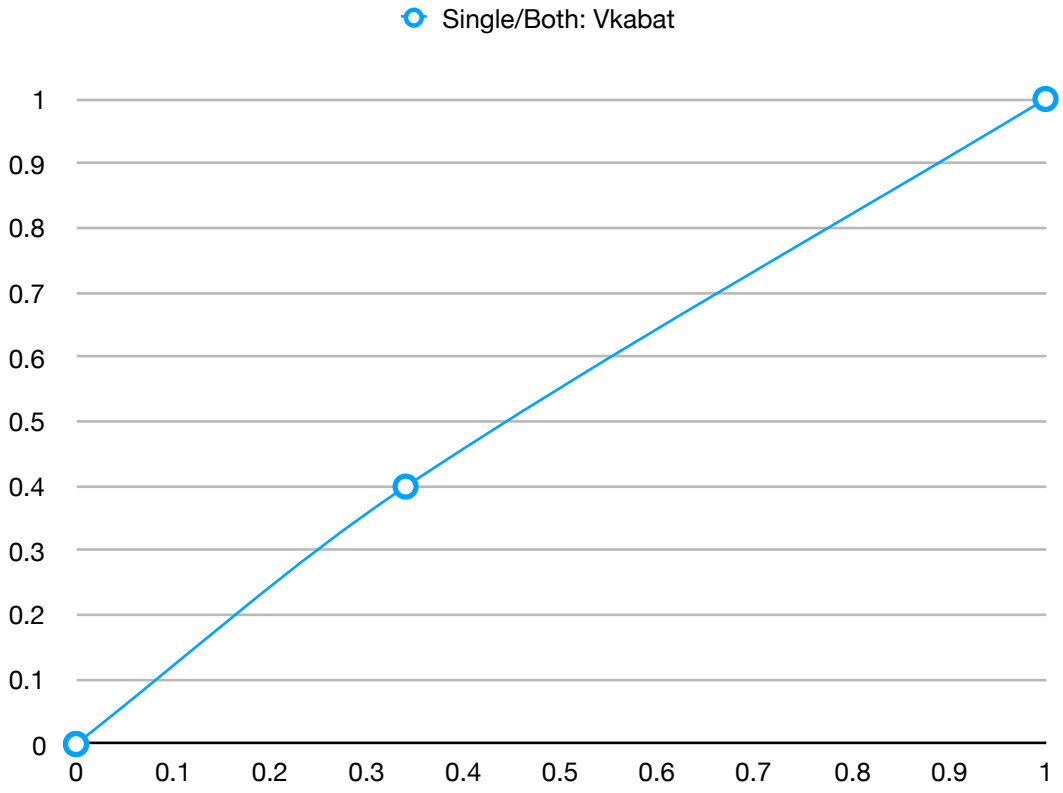
0.6
0.7
0.8
0.9
1


Single/Both: Vkabat
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0.2
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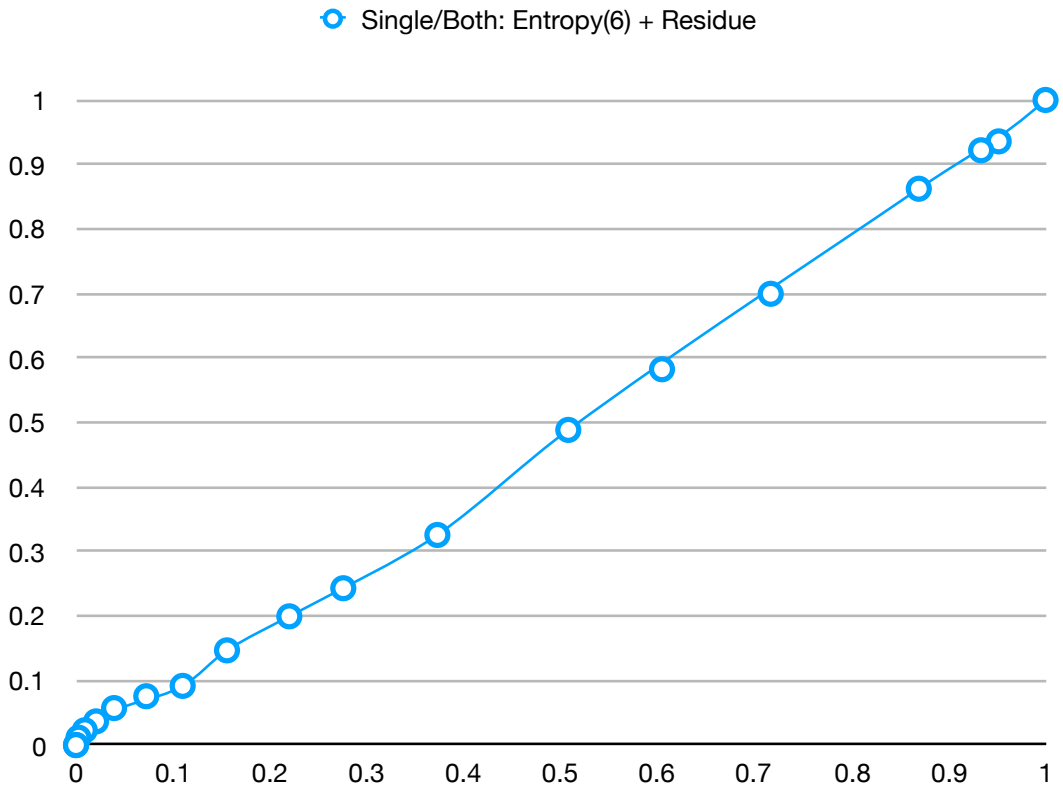
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1


Single/Both: Entropy(6) + Residue
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0.7
0.6
0.5
0.4
0.3
0.2
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0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
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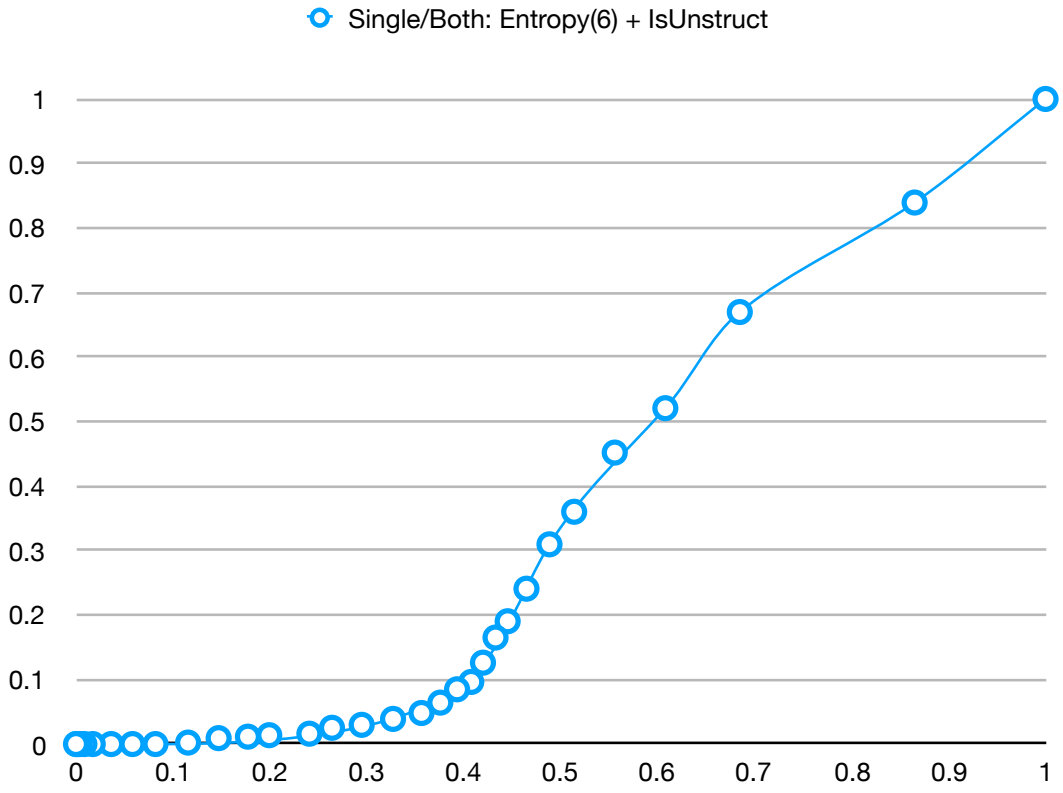
Single/Both: Entropy(6) + IsUnstruct
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0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
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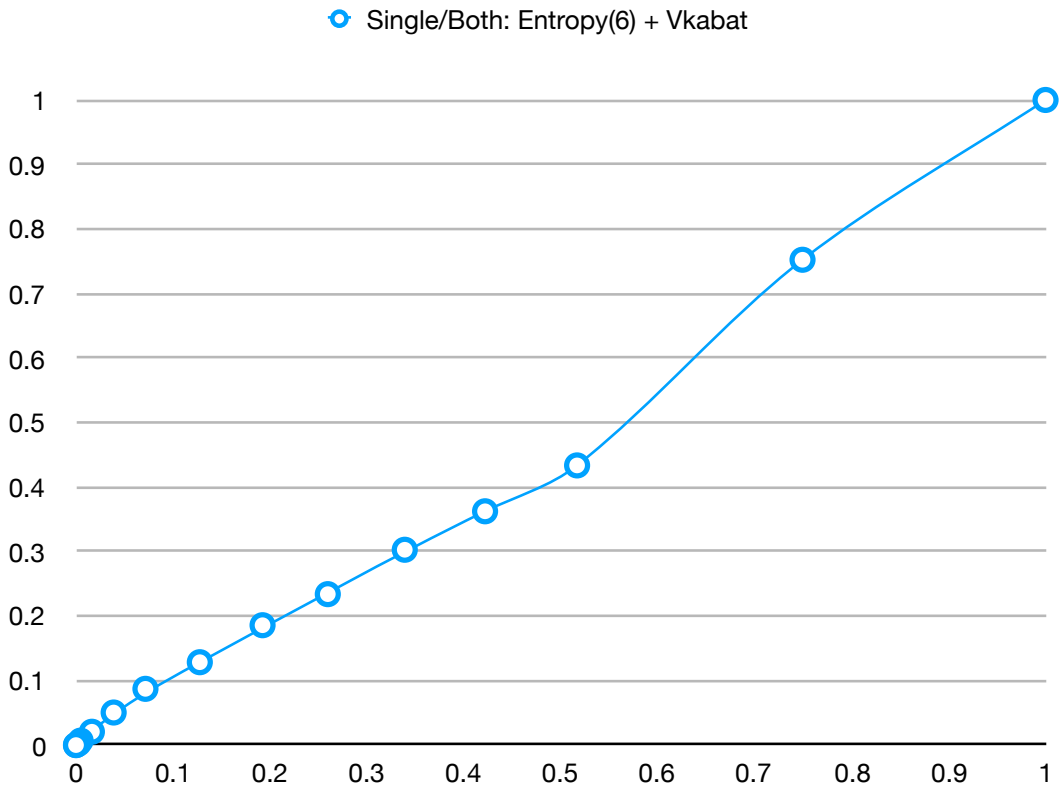
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1


Single/Both: Entropy(6) + Vkabat
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0.9
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0.4
0.3
0.2
0.1
0
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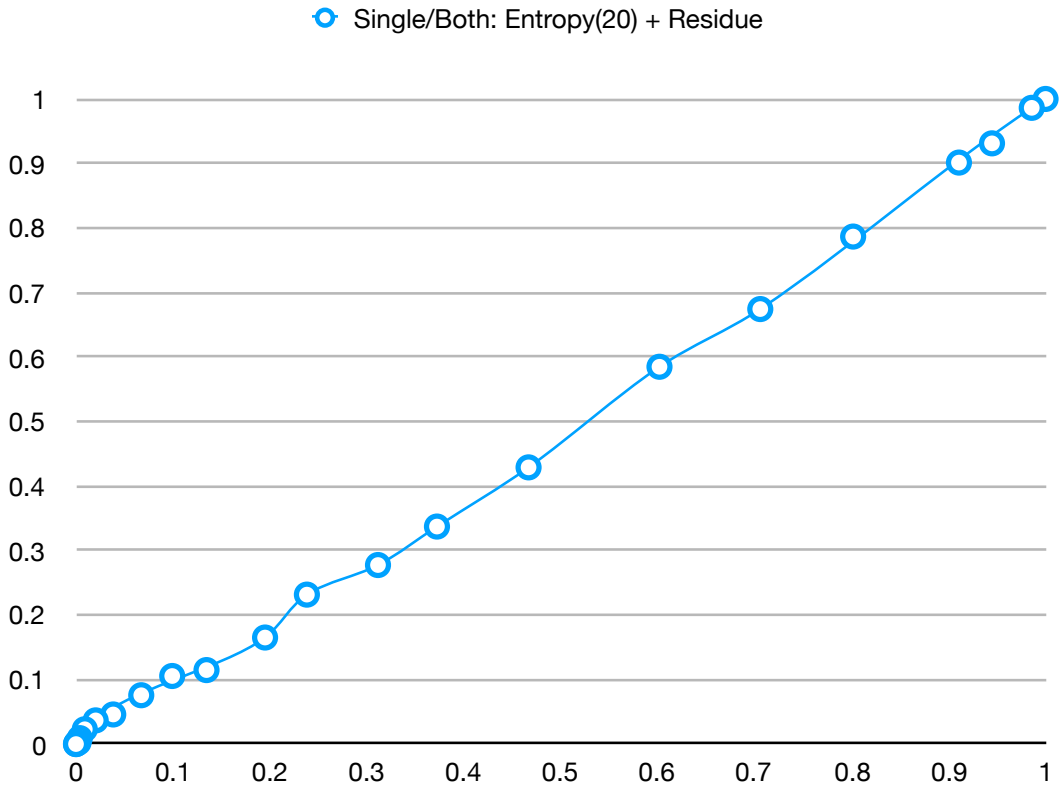
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1


Single/Both: Entropy(20) + Residue
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
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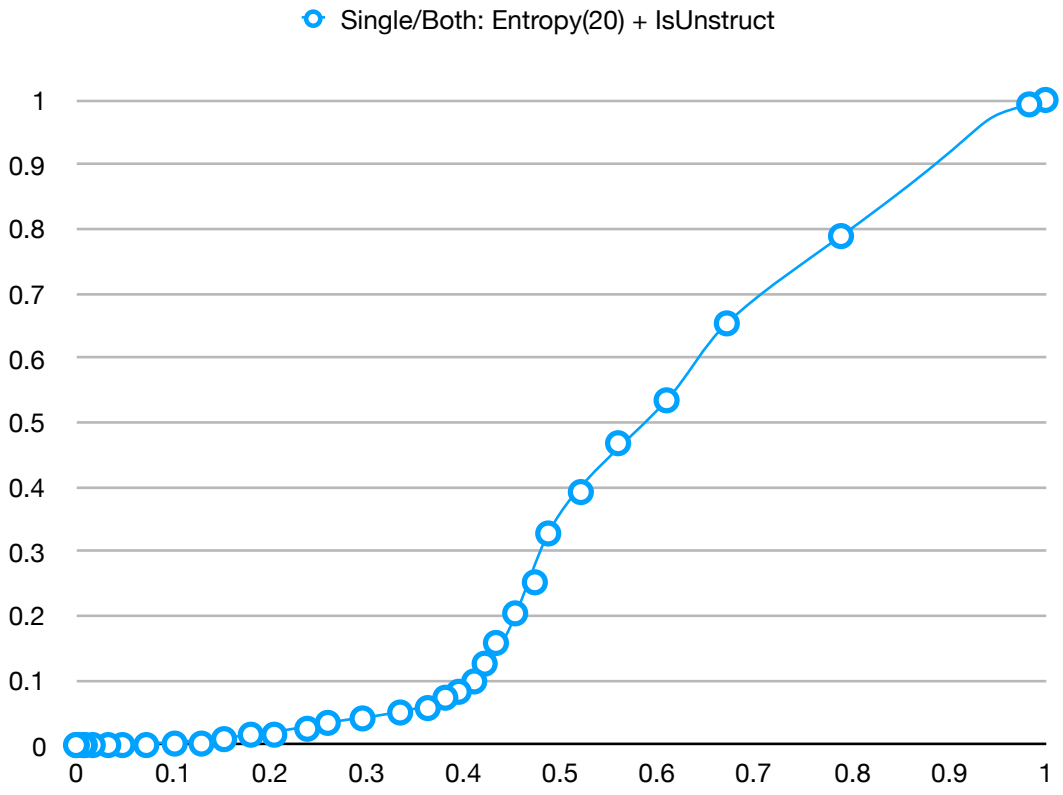
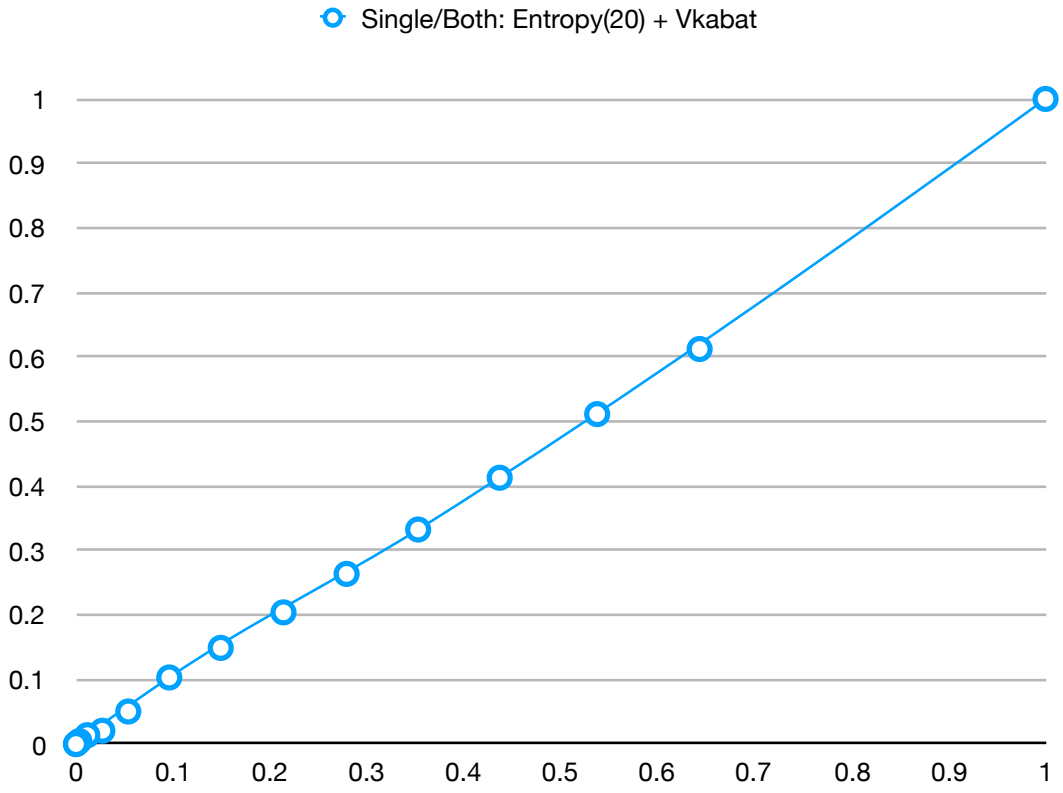
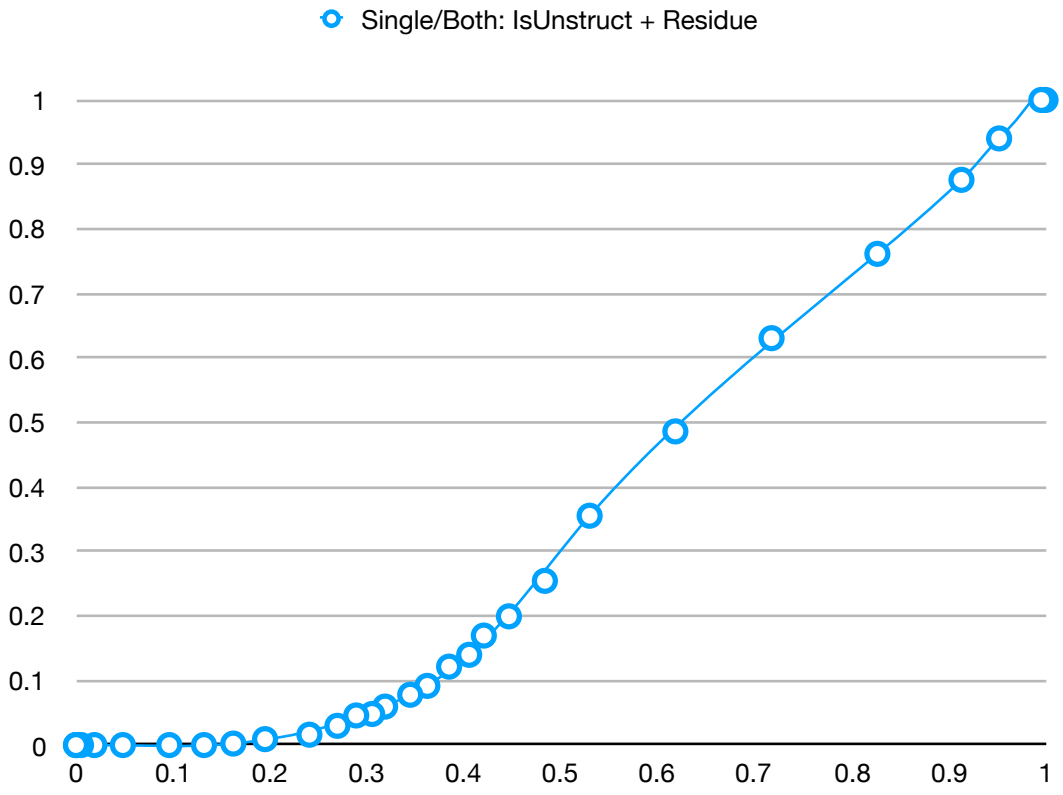
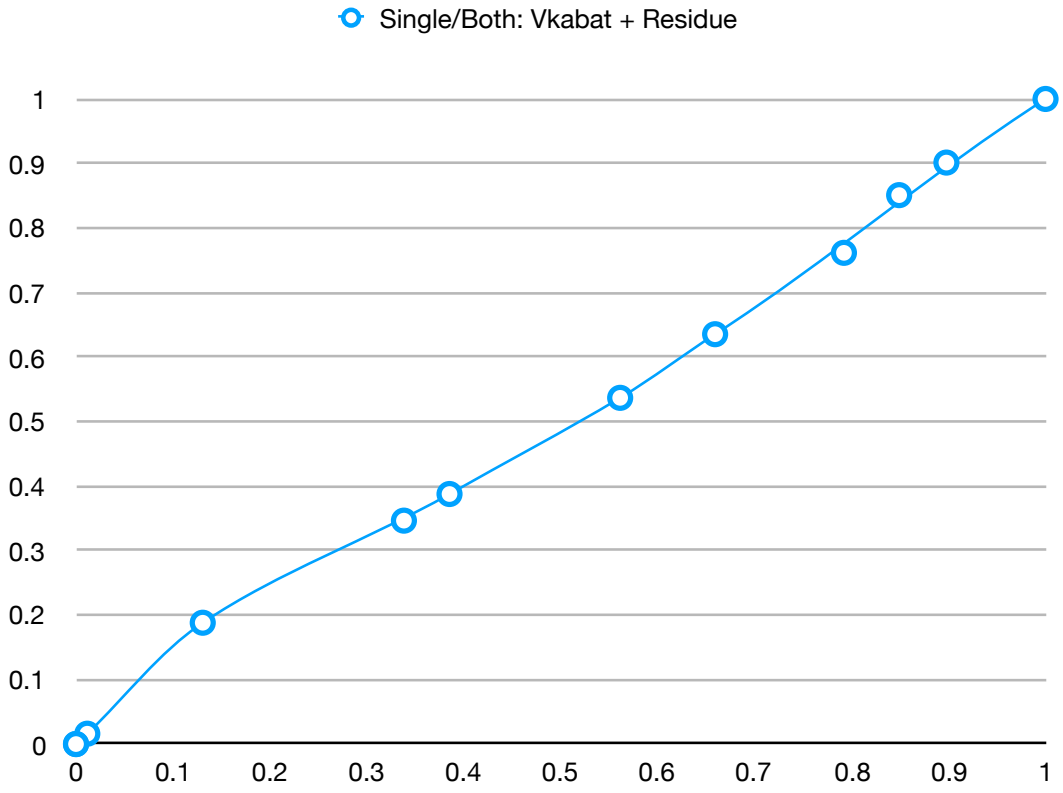
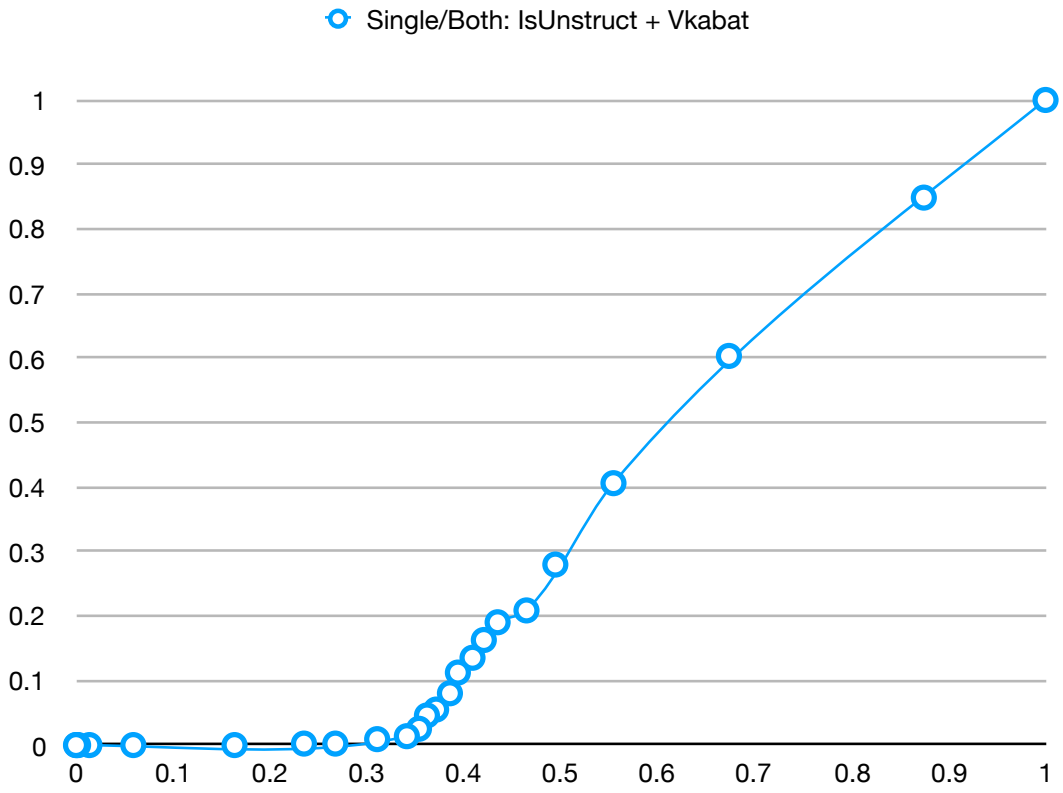
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

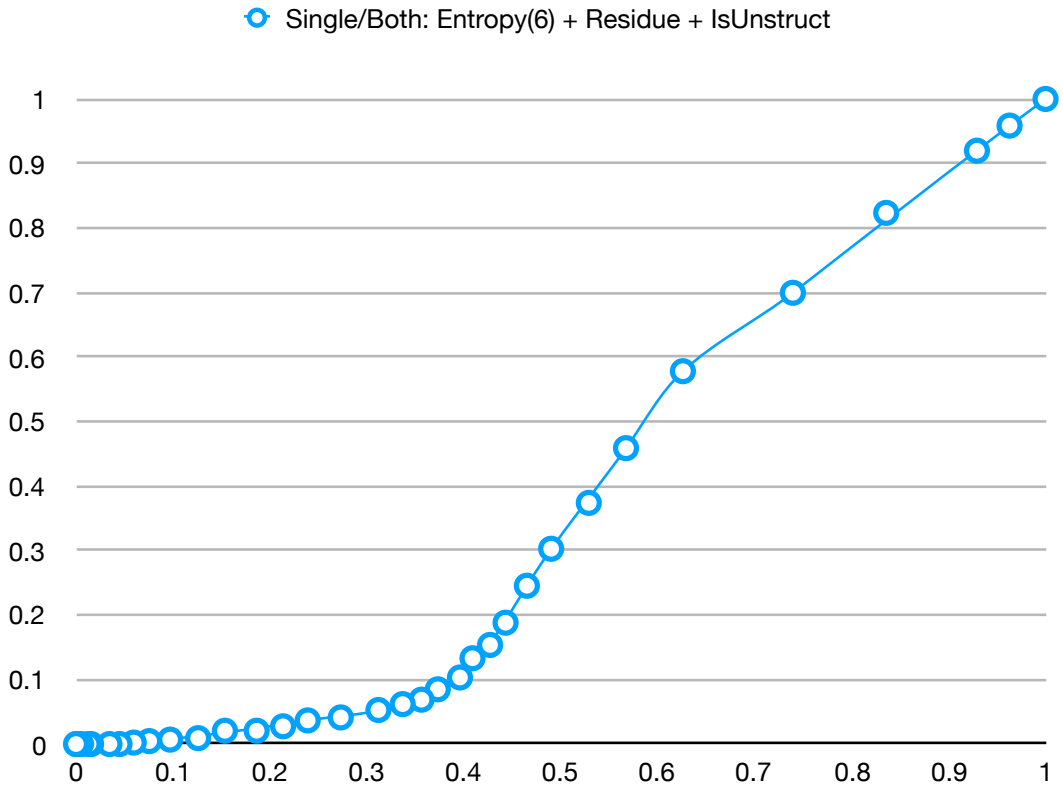

Single/Both: Entropy(20) + IsUnstruct
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1


Single/Both: Entropy(20) + Vkabat
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1


Single/Both: IsUnstruct + Residue
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1


Single/Both: Vkabat + Residue
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1


Single/Both: IsUnstruct + Vkabat
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1


Single/Both: Entropy(6) + Residue + IsUnstruct
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
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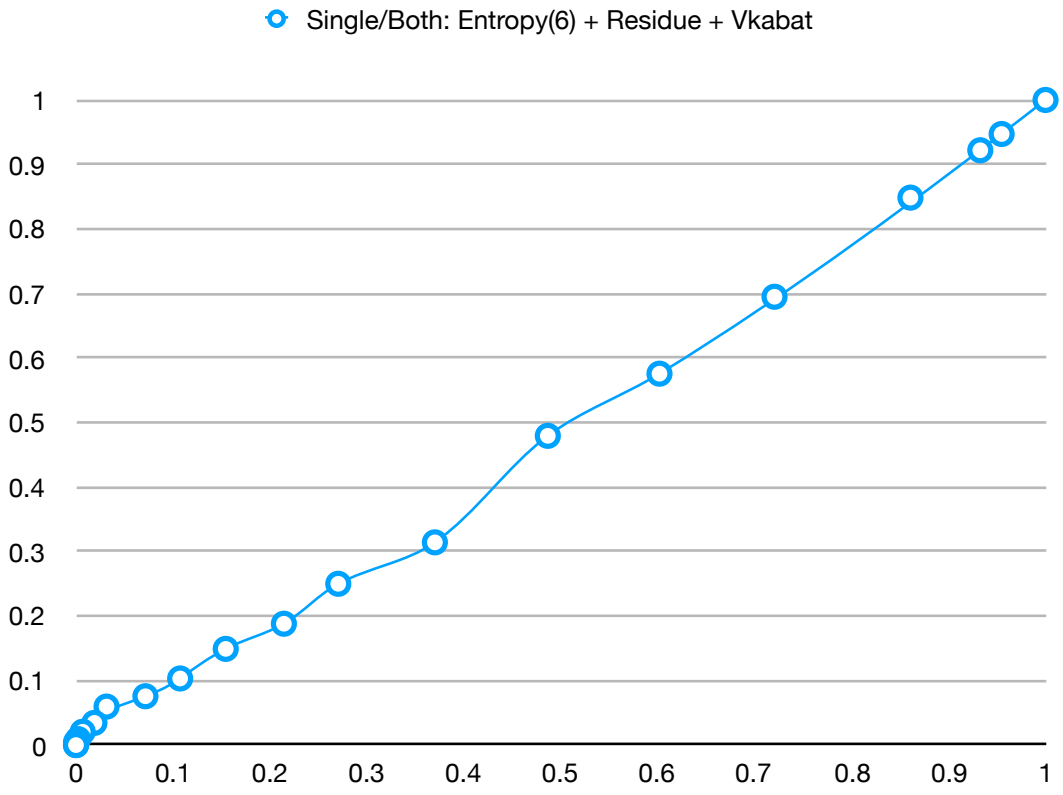
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1


Single/Both: Entropy(6) + Residue + Vkabat
1
0.9
0.8
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0.2
0.1
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0.1
0.2
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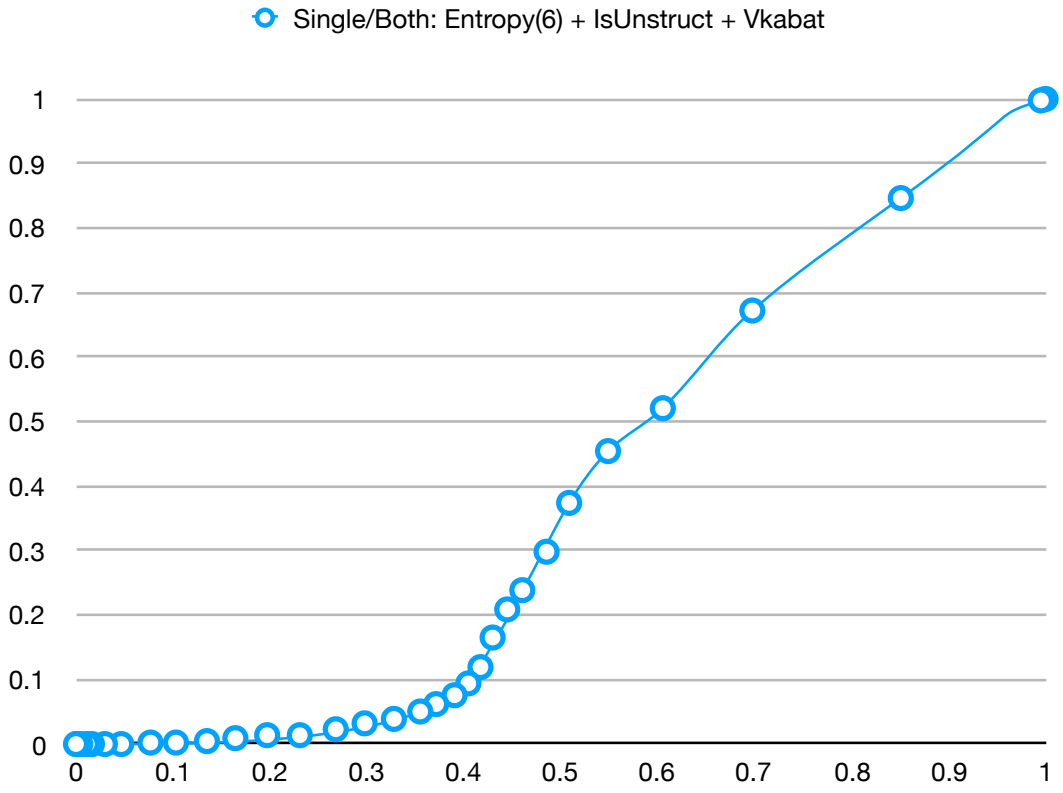
0.4
0.5
0.6
0.7
0.8
0.9
1


Single/Both: Entropy(6) + IsUnstruct + Vkabat
1
0.9
0.8
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0.5
0.4
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0.2
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0.1
0.2
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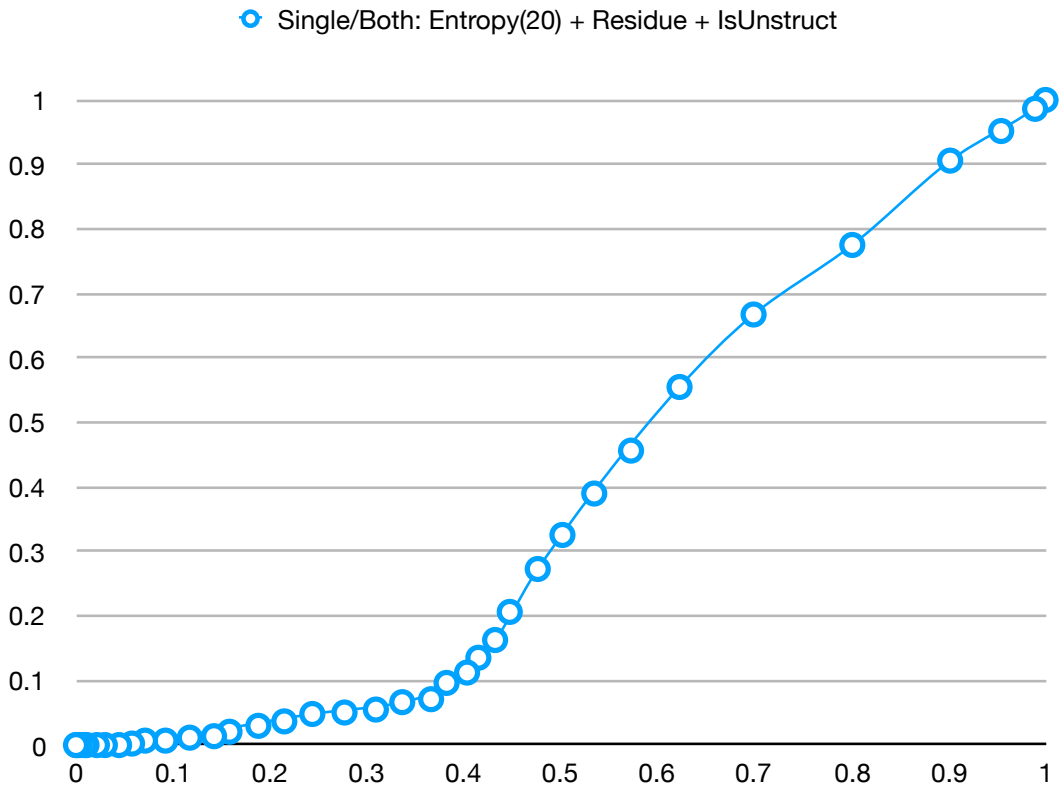
0.4
0.5
0.6
0.7
0.8
0.9
1


Single/Both: Entropy(20) + Residue + IsUnstruct
1
0.9
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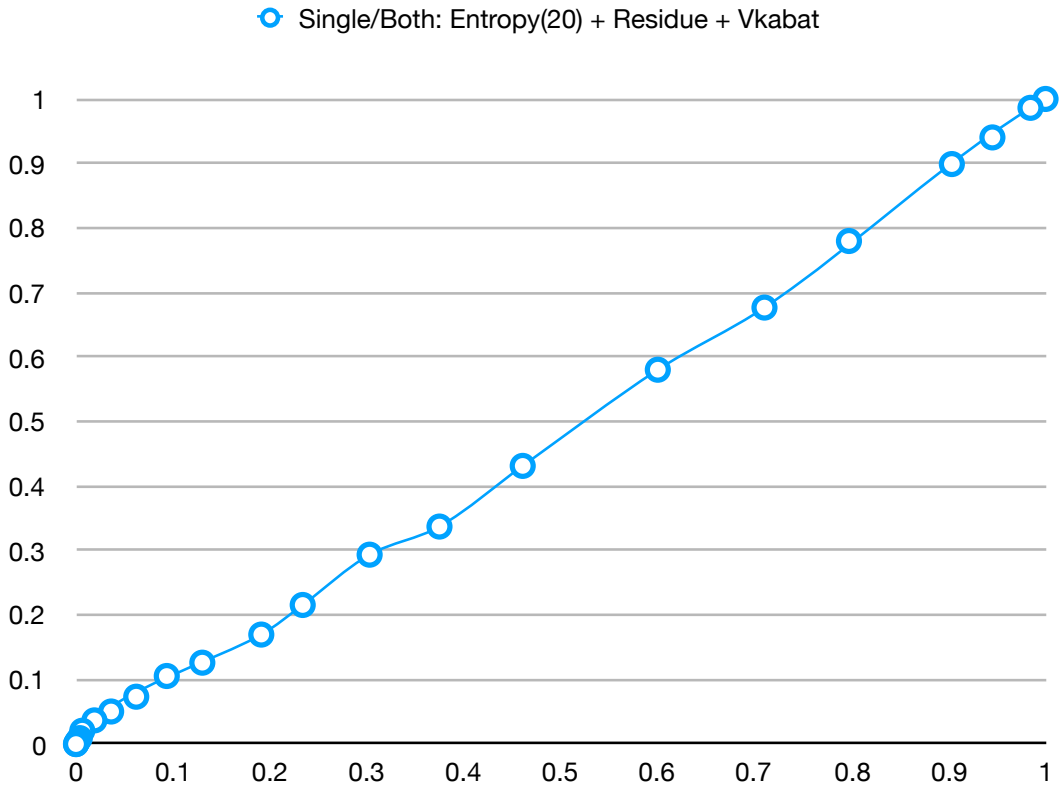
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1


Single/Both: Entropy(20) + Residue + Vkabat
1
0.9
0.8
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0.5
0.4
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0.2
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0.1
0.2
0.3
0.4
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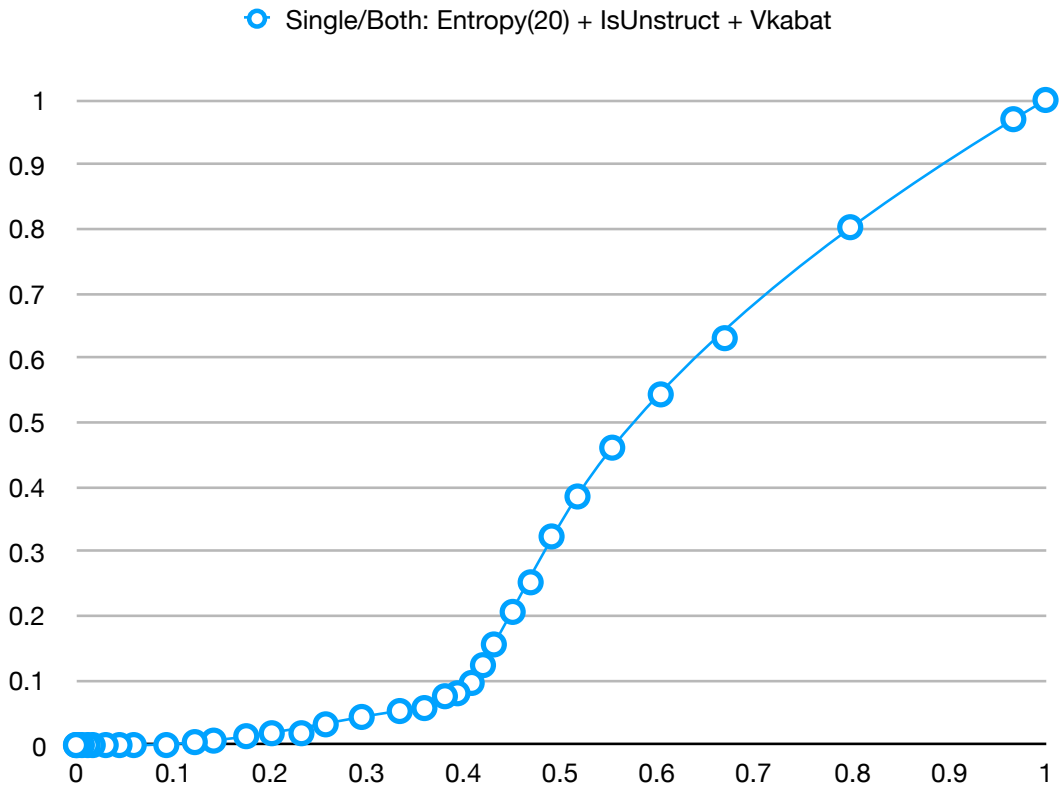
0.6
0.7
0.8
0.9
1


Single/Both: Entropy(20) + IsUnstruct + Vkabat
1
0.9
0.8
0.7
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0.3
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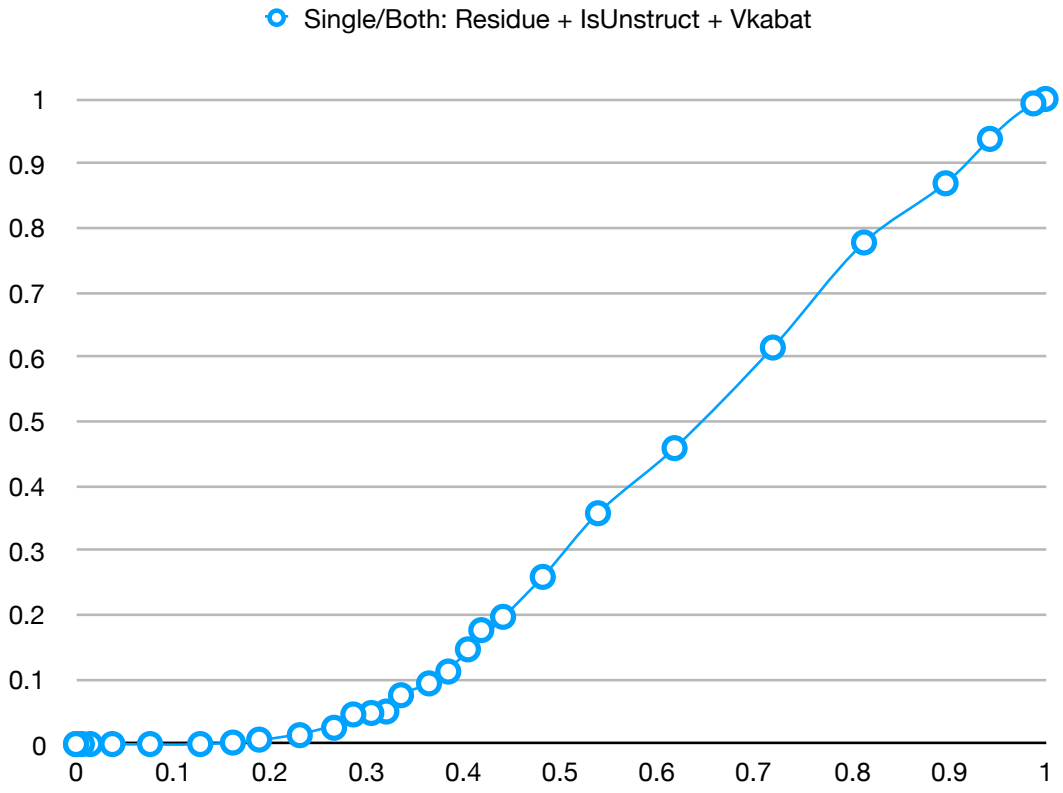
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1


Single/Both: Residue + IsUnstruct + Vkabat
1
0.9
0.8
0.7
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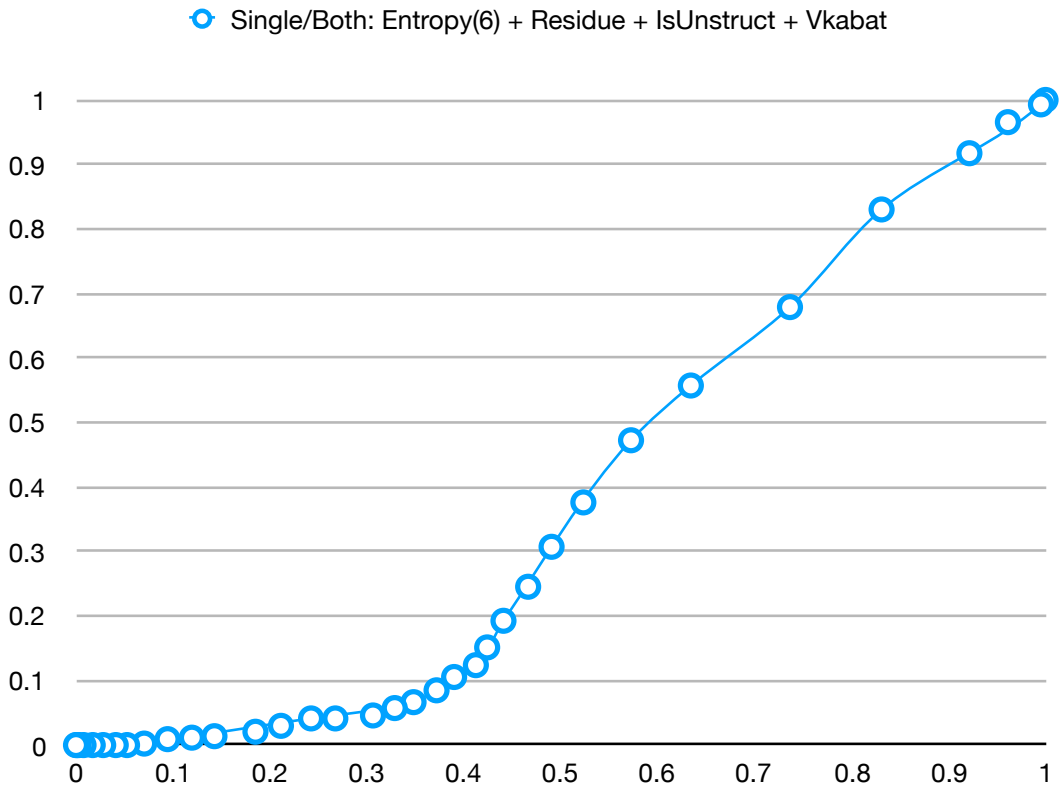
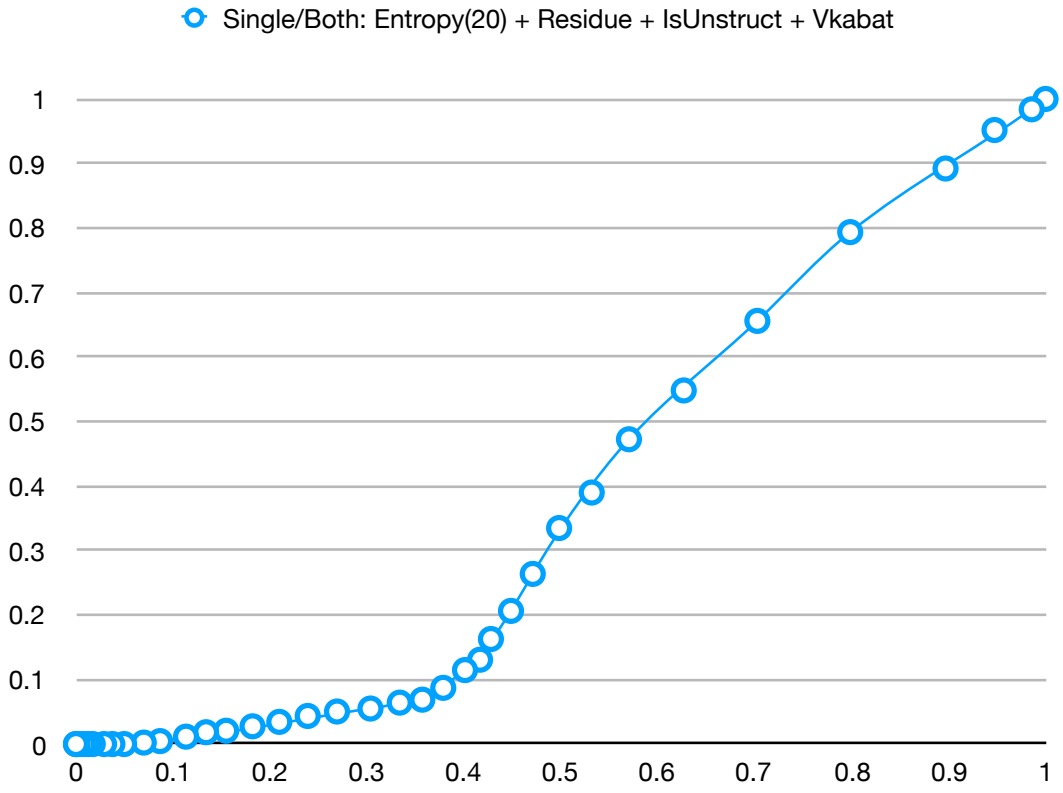
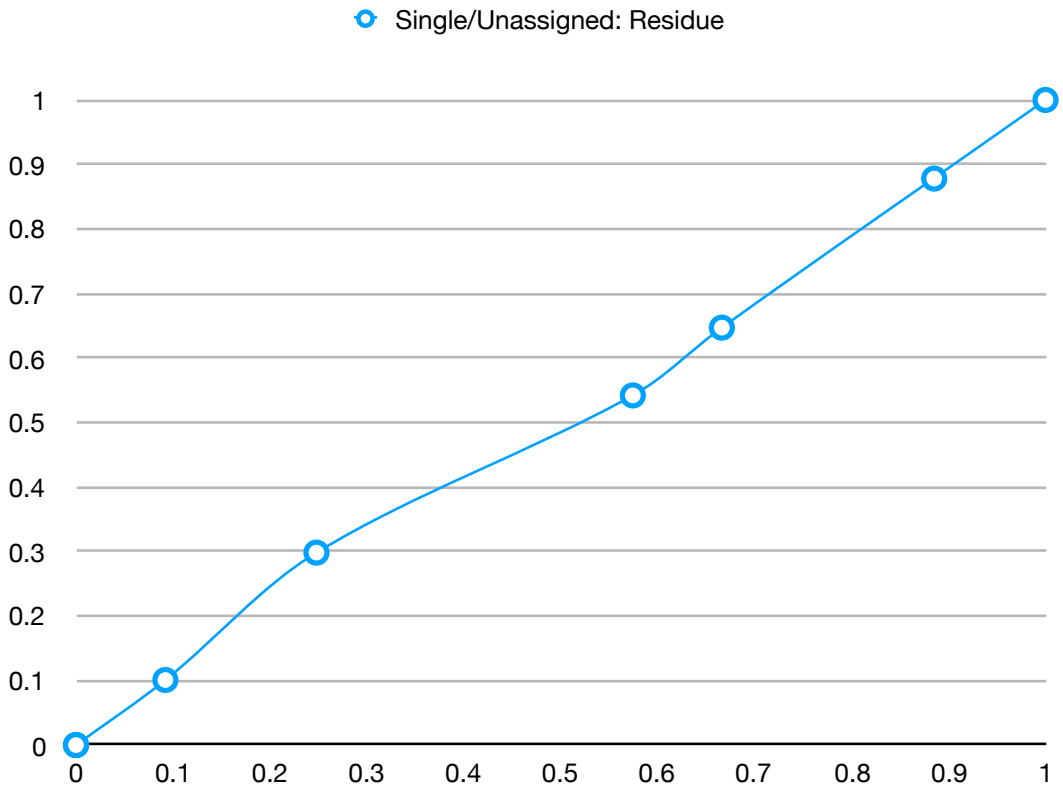
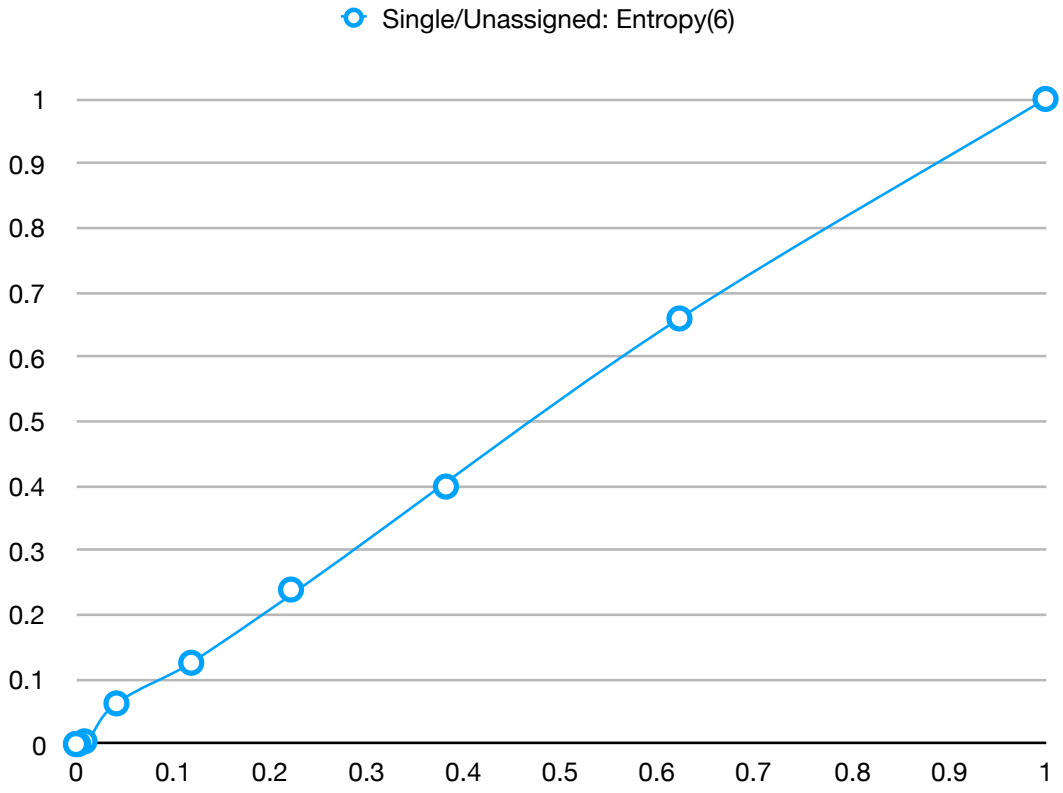
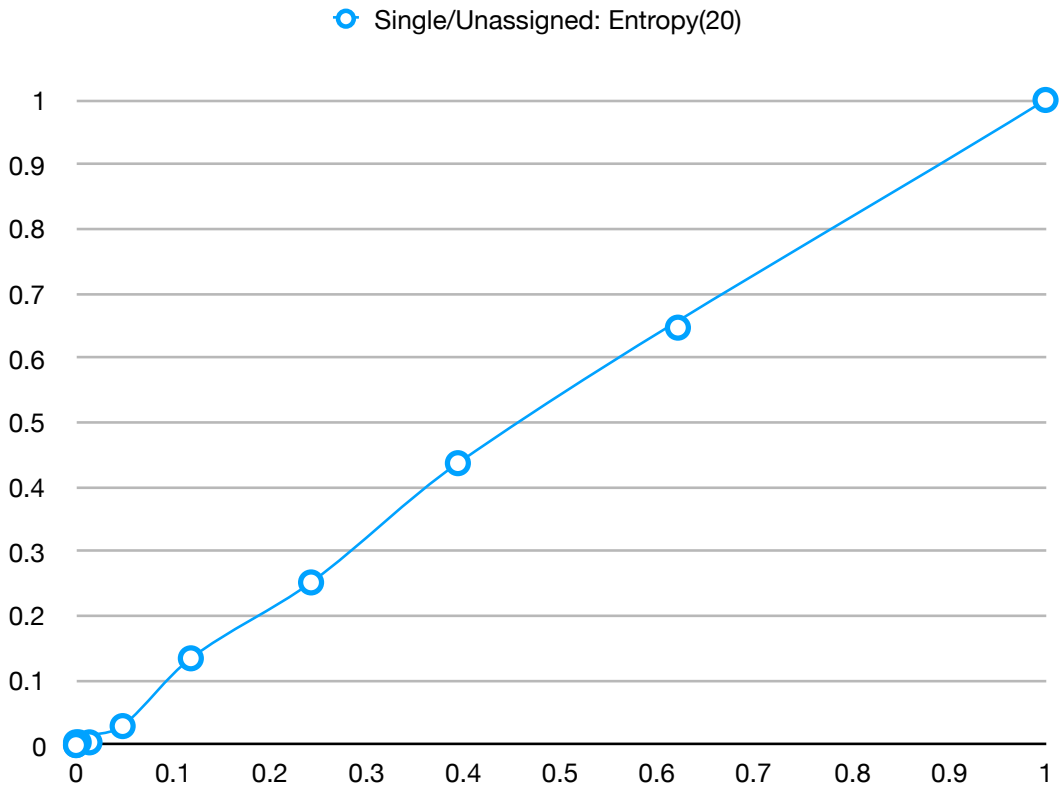
0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

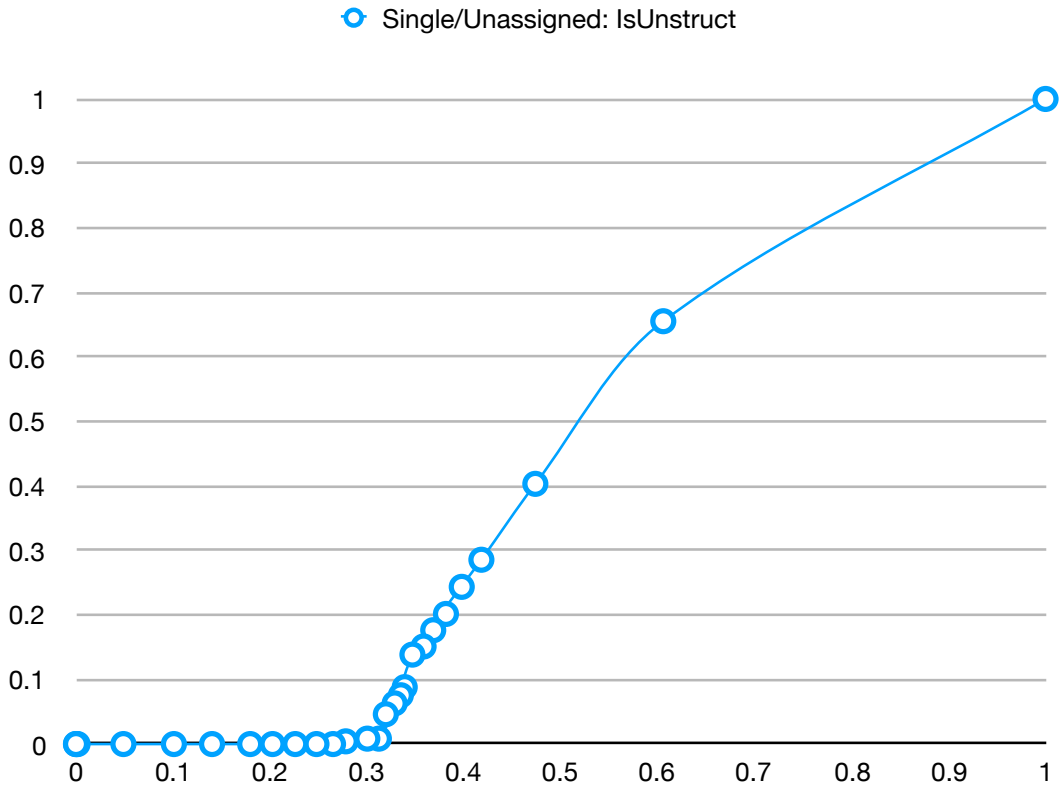

Single/Both: Entropy(6) + Residue + IsUnstruct + Vkabat
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

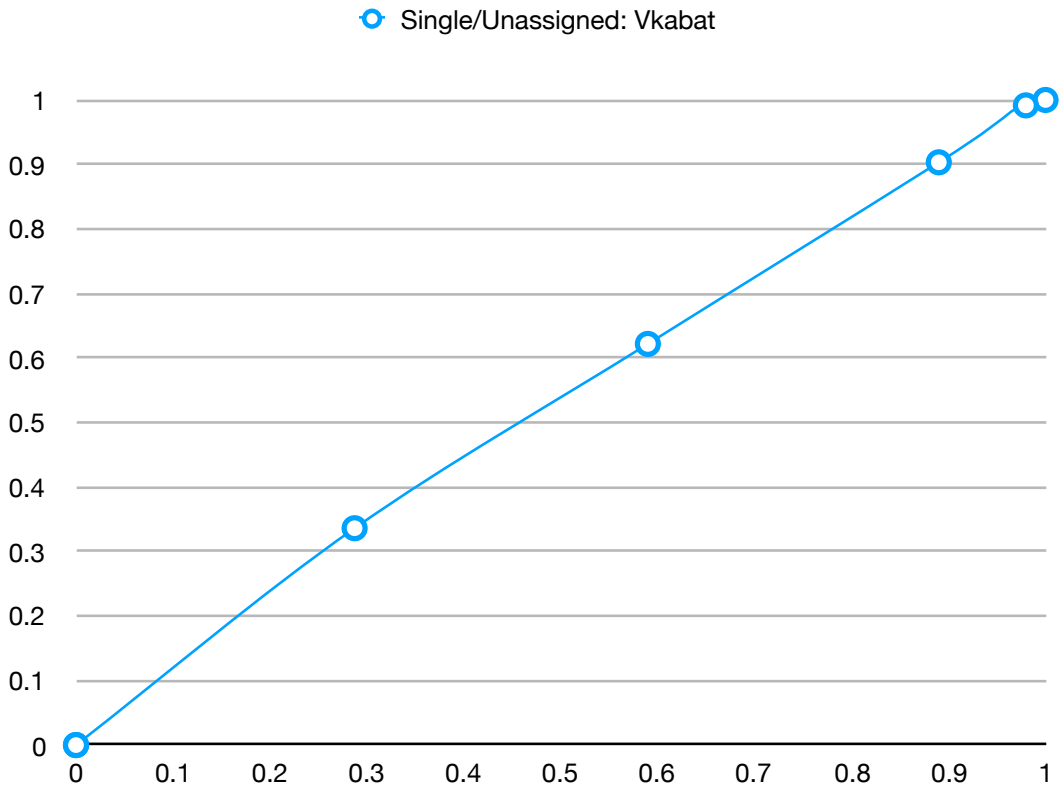

Single/Both: Entropy(20) + Residue + IsUnstruct + Vkabat
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

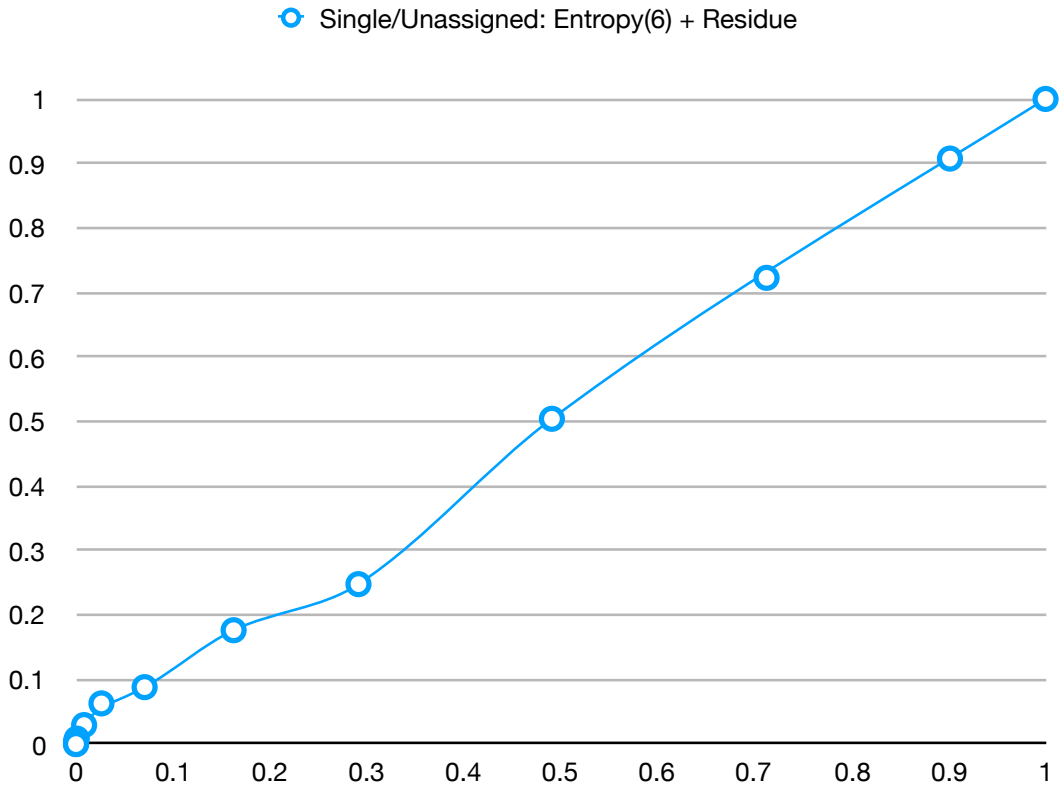

Single/Unassigned: Residue
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

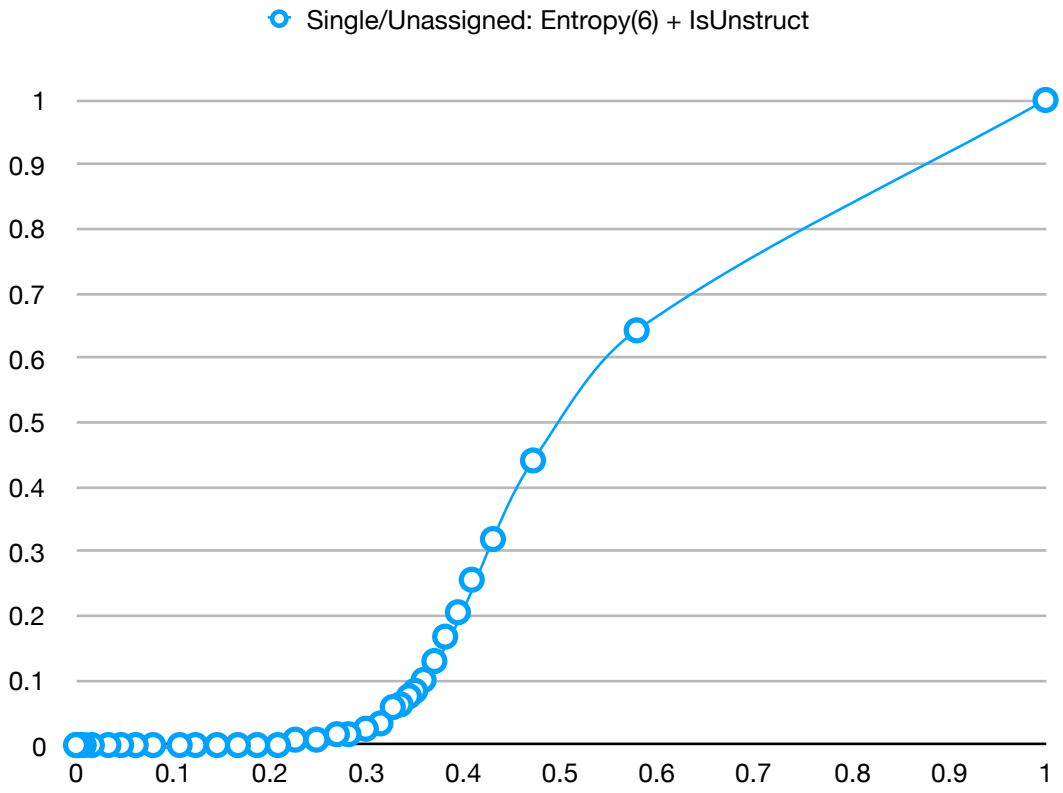

Single/Unassigned: Entropy(6)
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

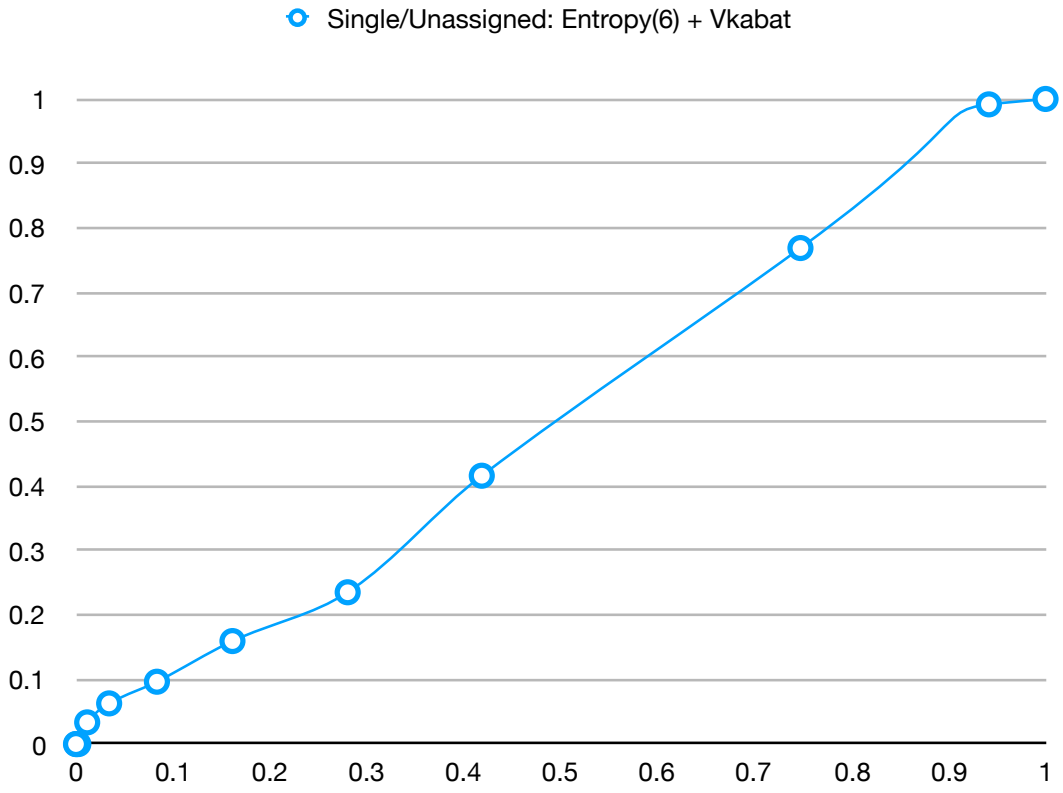

Single/Unassigned: Entropy(20)
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

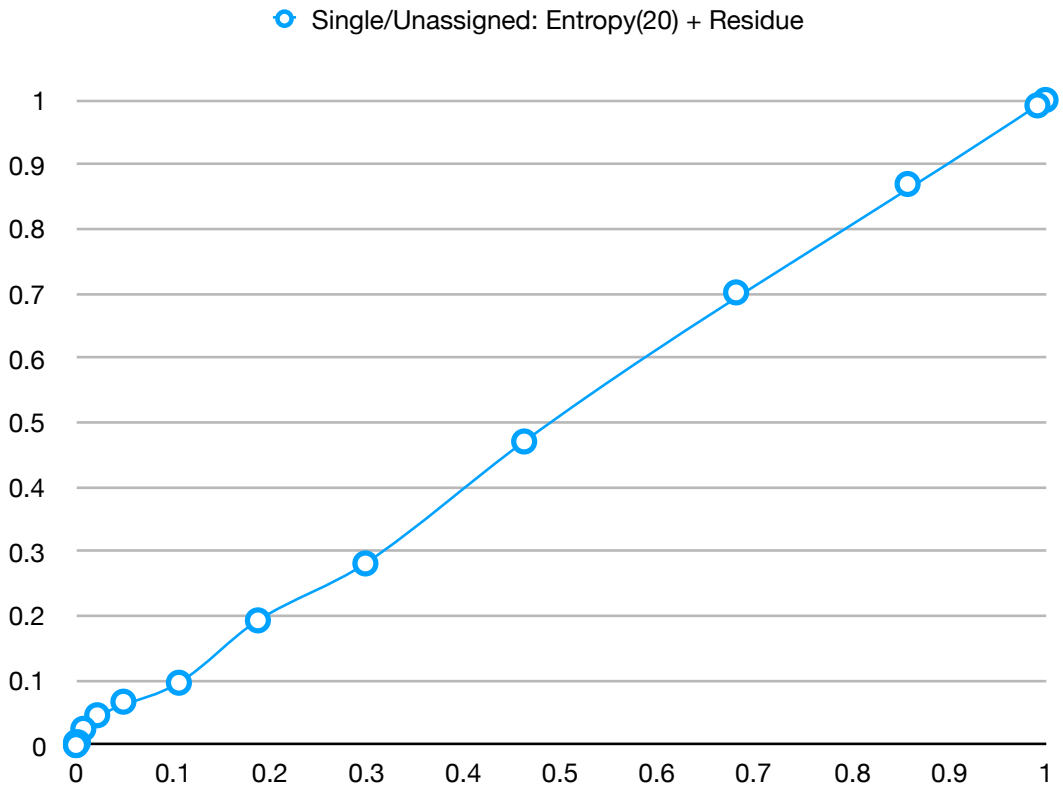

Single/Unassigned: IsUnstruct
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

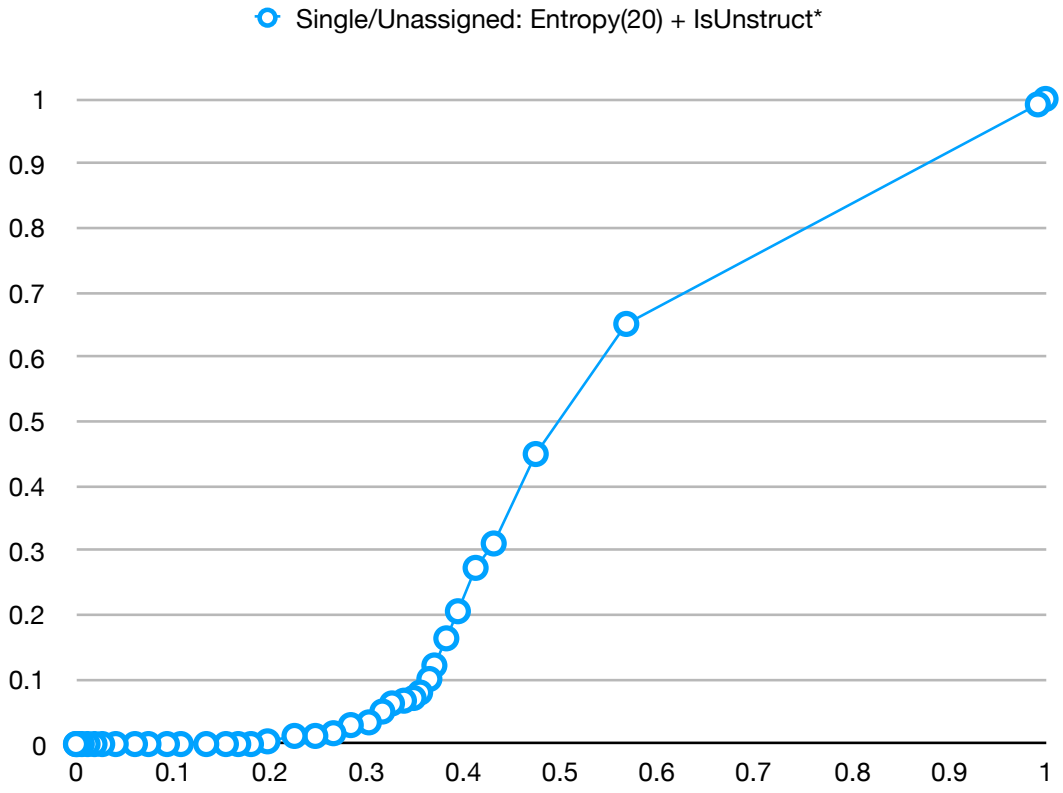

Single/Unassigned: Vkabat
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1


Single/Unassigned: Entropy(6) + Residue
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1


Single/Unassigned: Entropy(6) + IsUnstruct
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1


Single/Unassigned: Entropy(6) + Vkabat
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1


Single/Unassigned: Entropy(20) + Residue
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1


Single/Unassigned: Entropy(20) + IsUnstruct*
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
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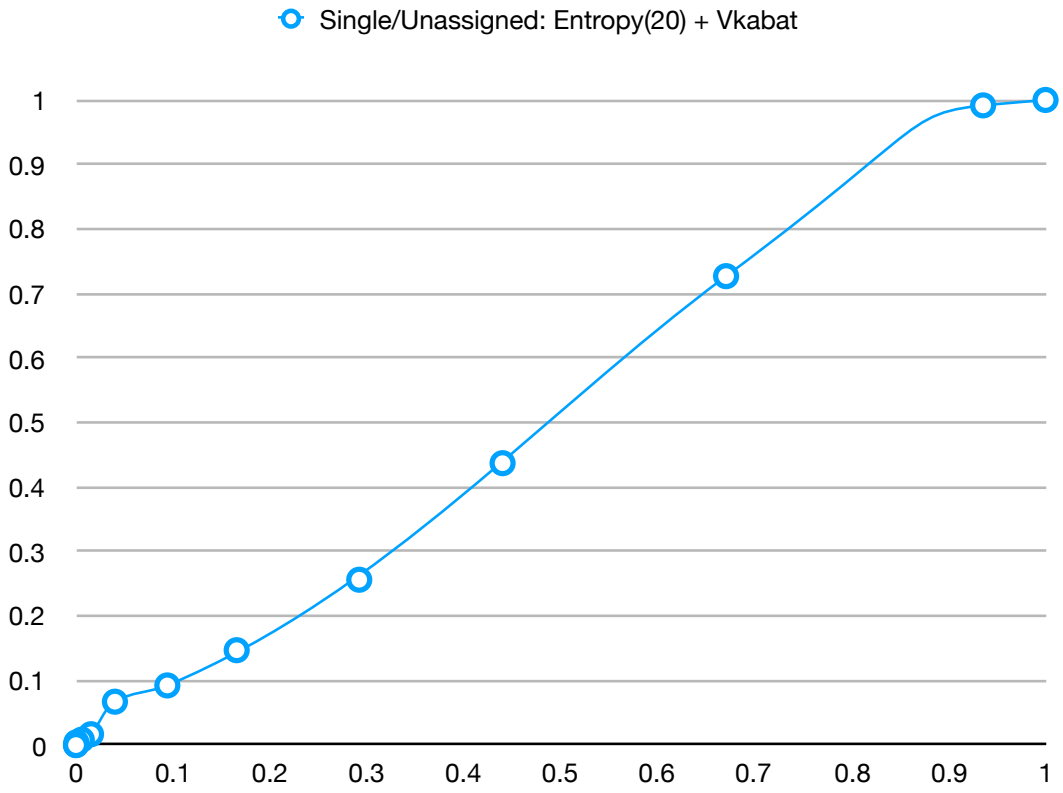
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1


Single/Unassigned: Entropy(20) + Vkabat
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
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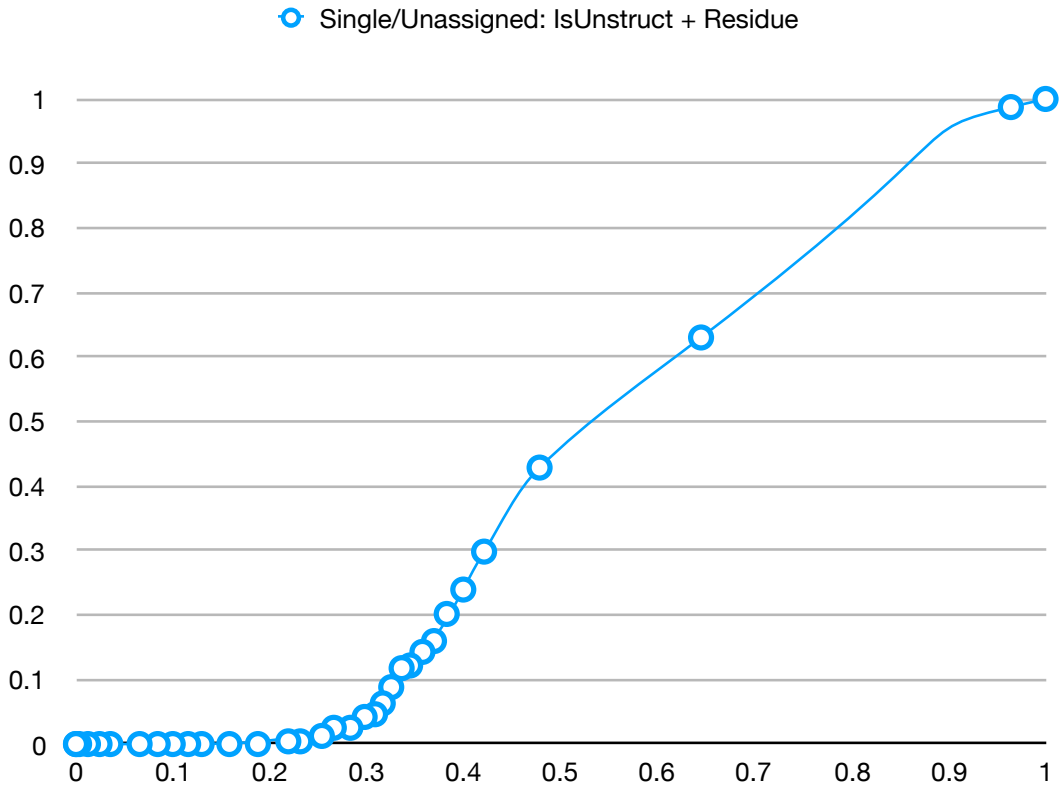
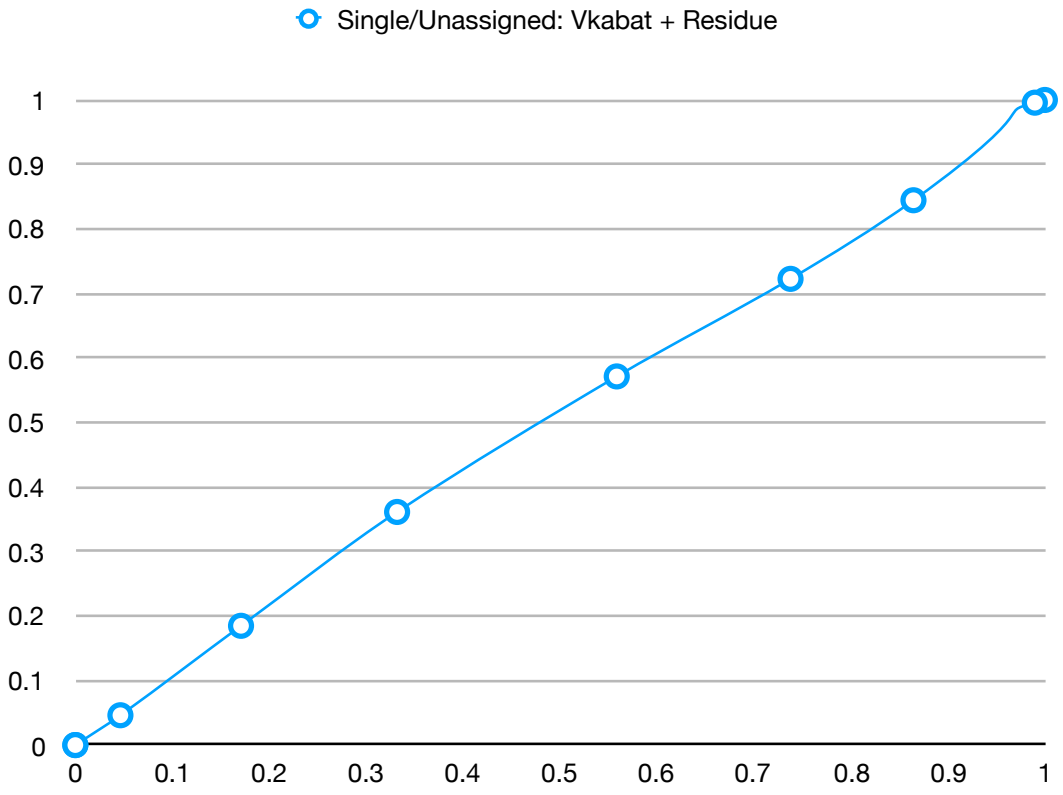
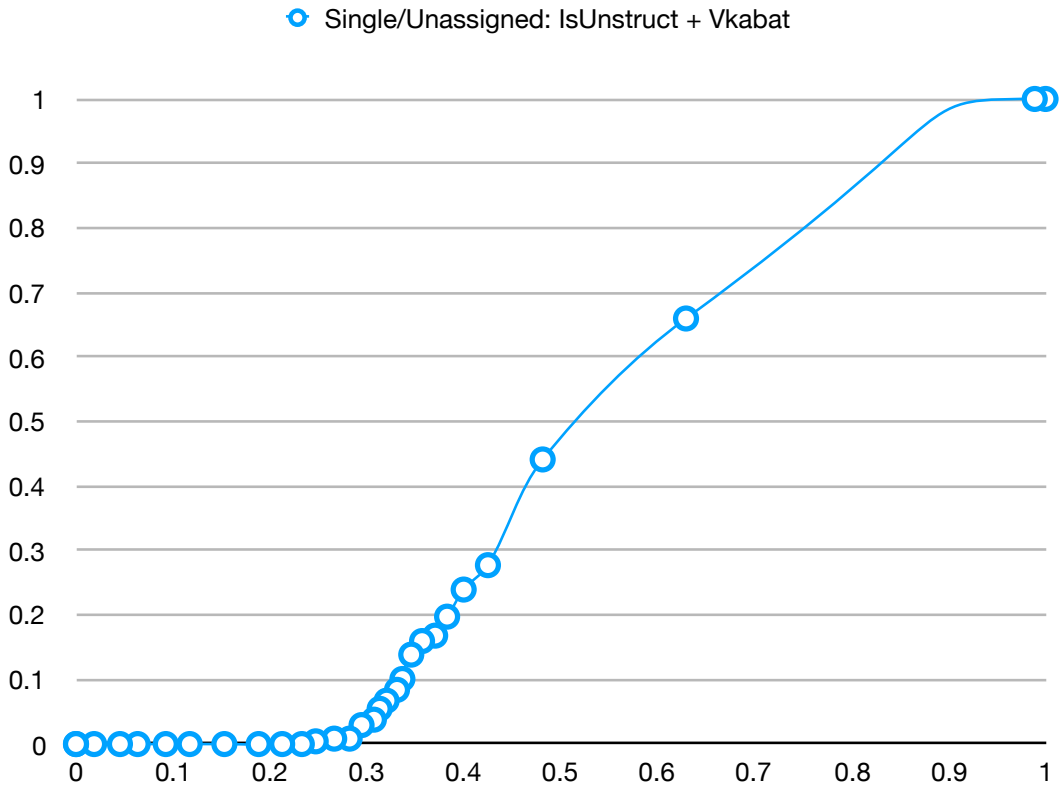
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1


Single/Unassigned: IsUnstruct + Residue
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1


Single/Unassigned: Vkabat + Residue
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1


Single/Unassigned: IsUnstruct + Vkabat
1
0.9
0.8
0.7
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0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
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0.4
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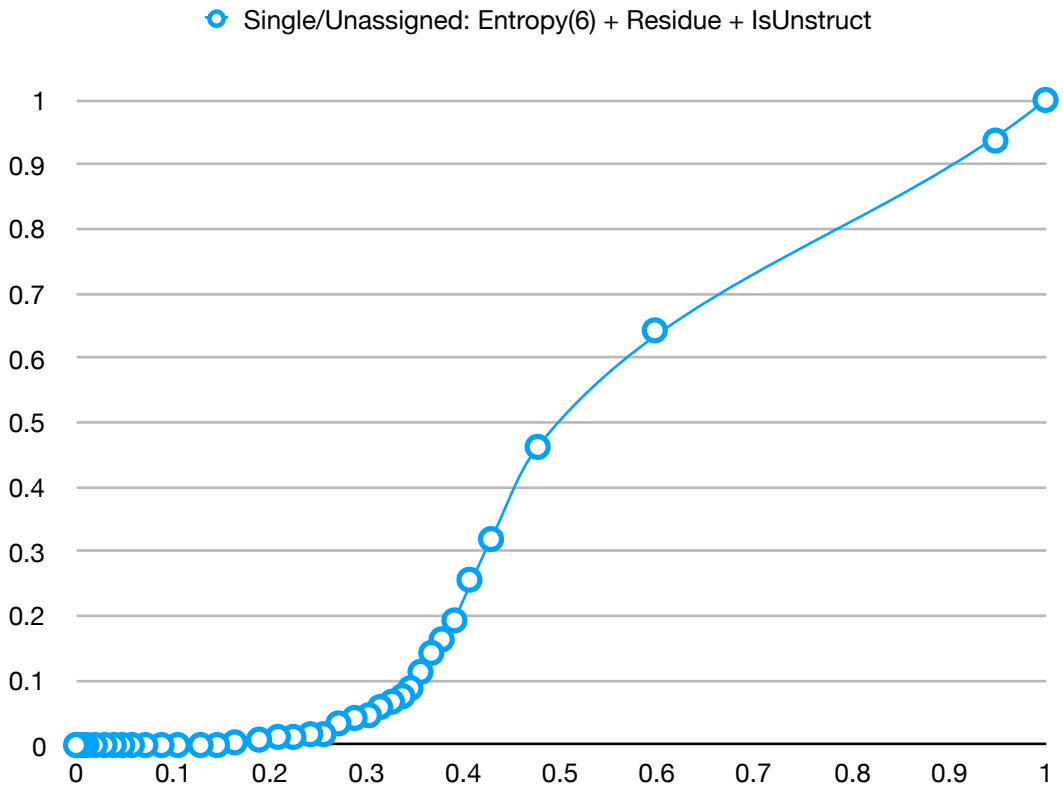
0.6
0.7
0.8
0.9
1


Single/Unassigned: Entropy(6) + Residue + IsUnstruct
1
0.9
0.8
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0.1
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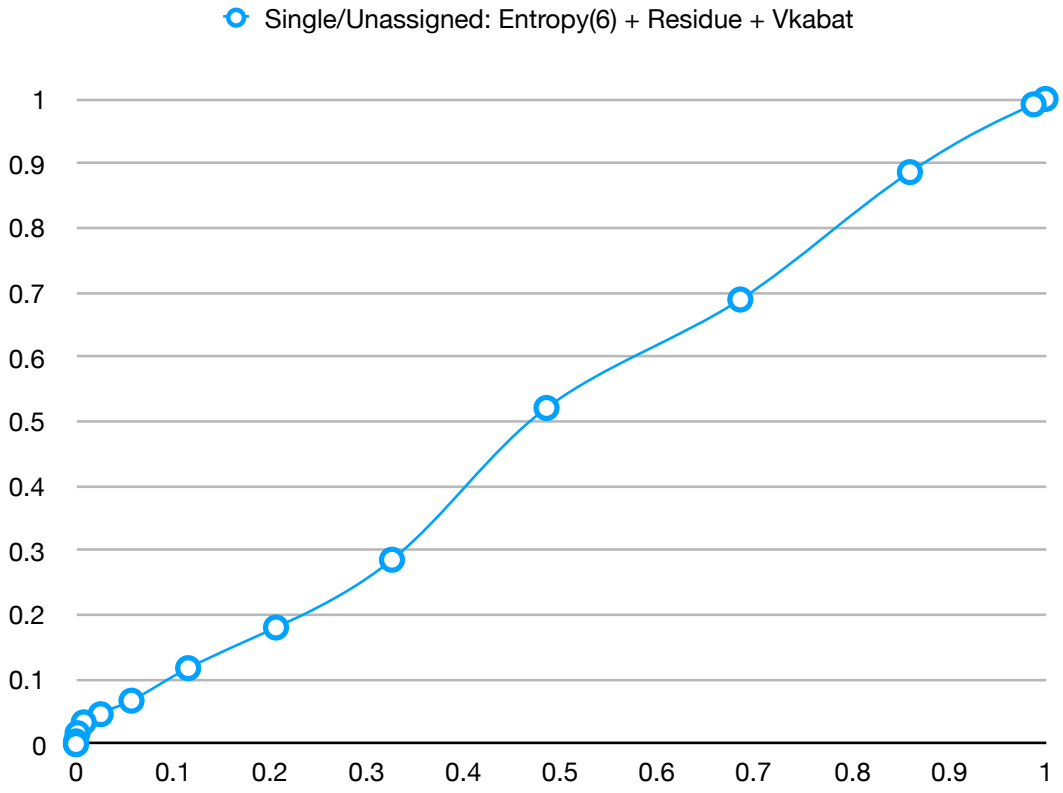
0.6
0.7
0.8
0.9
1


Single/Unassigned: Entropy(6) + Residue + Vkabat
1
0.9
0.8
0.7
0.6
0.5
0.4
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0.2
0.1
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0
0.1
0.2
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0.4
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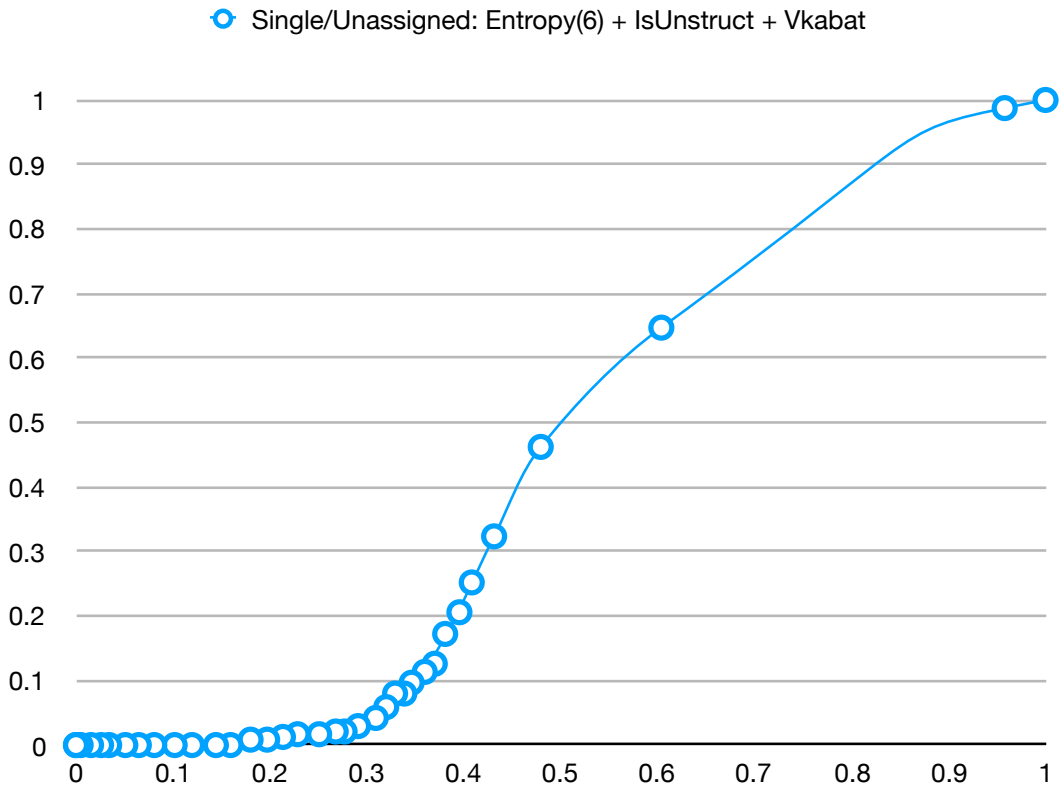
0.6
0.7
0.8
0.9
1


Single/Unassigned: Entropy(6) + IsUnstruct + Vkabat
1
0.9
0.8
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0.6
0.5
0.4
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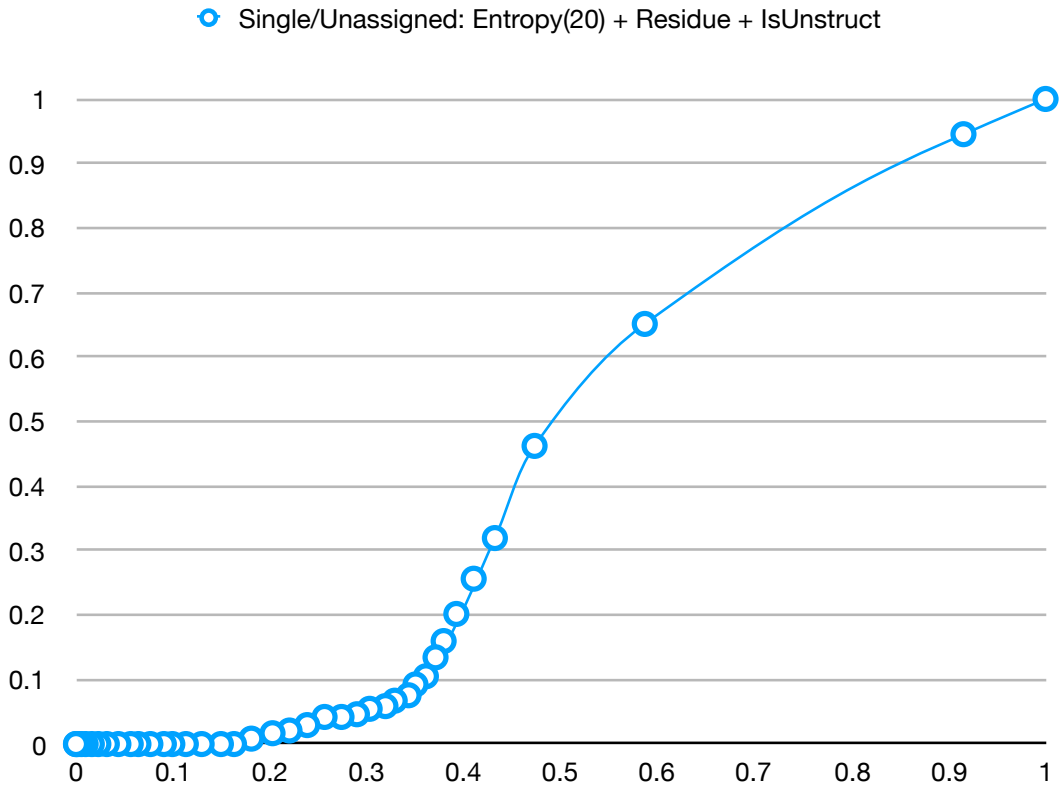
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1


Single/Unassigned: Entropy(20) + Residue + IsUnstruct
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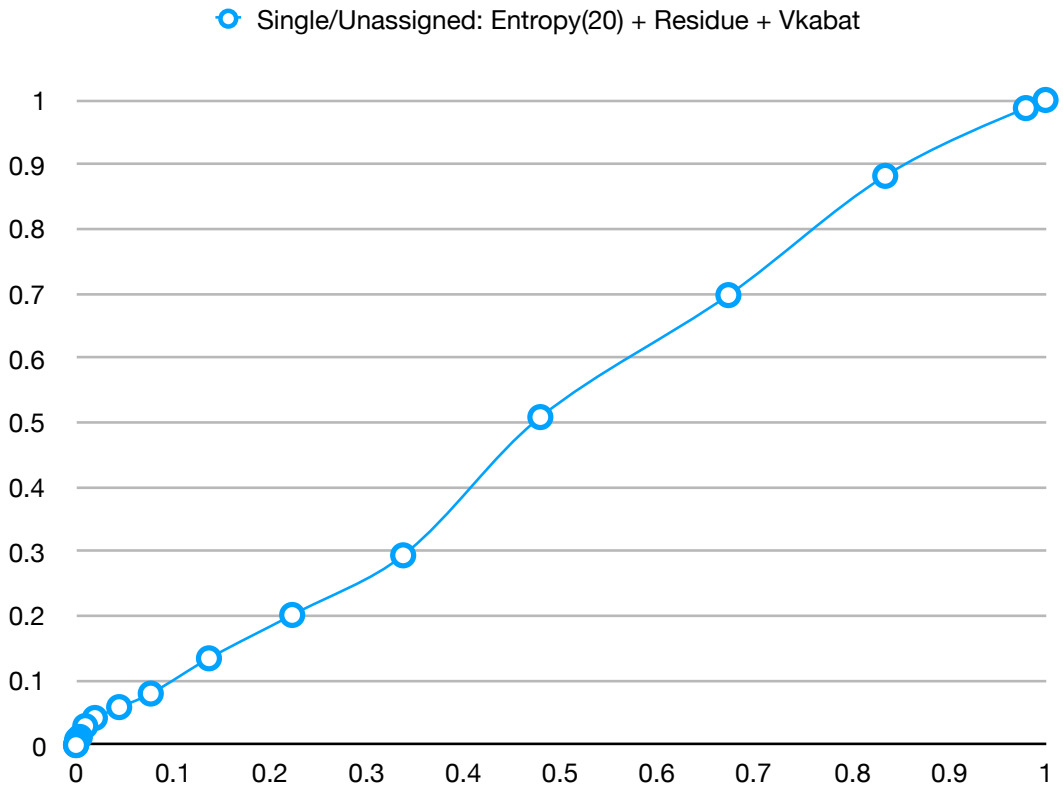
Single/Unassigned: Entropy(20) + Residue + Vkabat
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0.9
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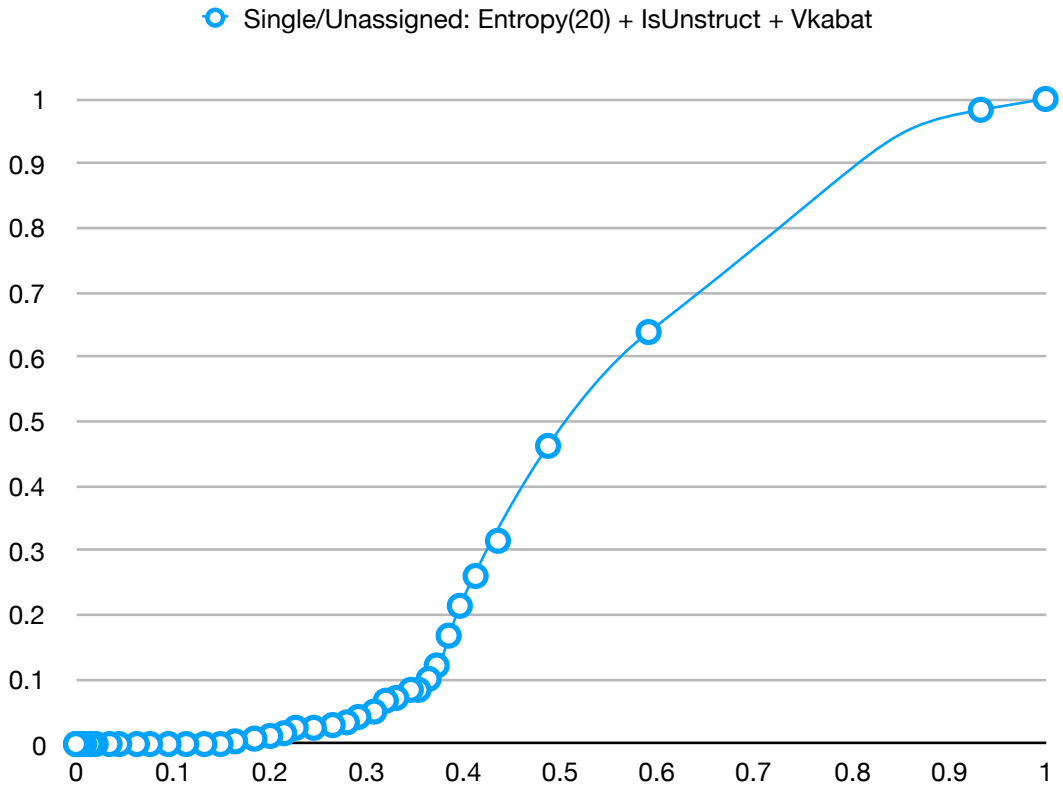
Single/Unassigned: Entropy(20) + IsUnstruct + Vkabat
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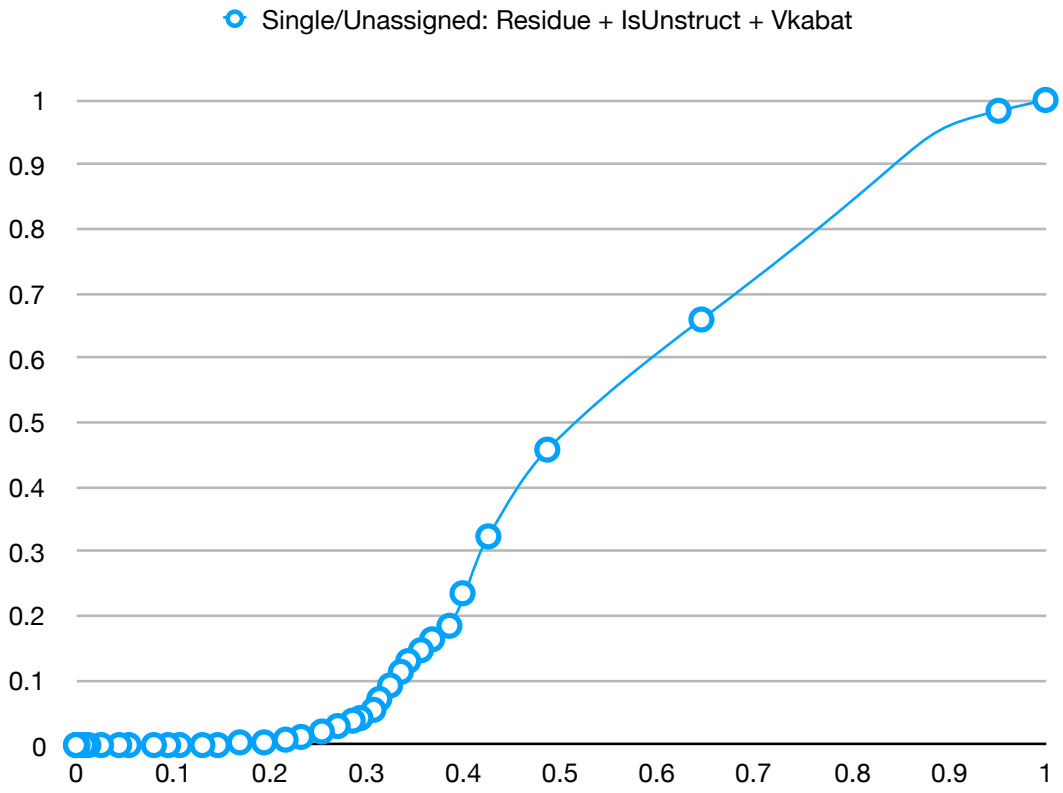
Single/Unassigned: Residue + IsUnstruct + Vkabat
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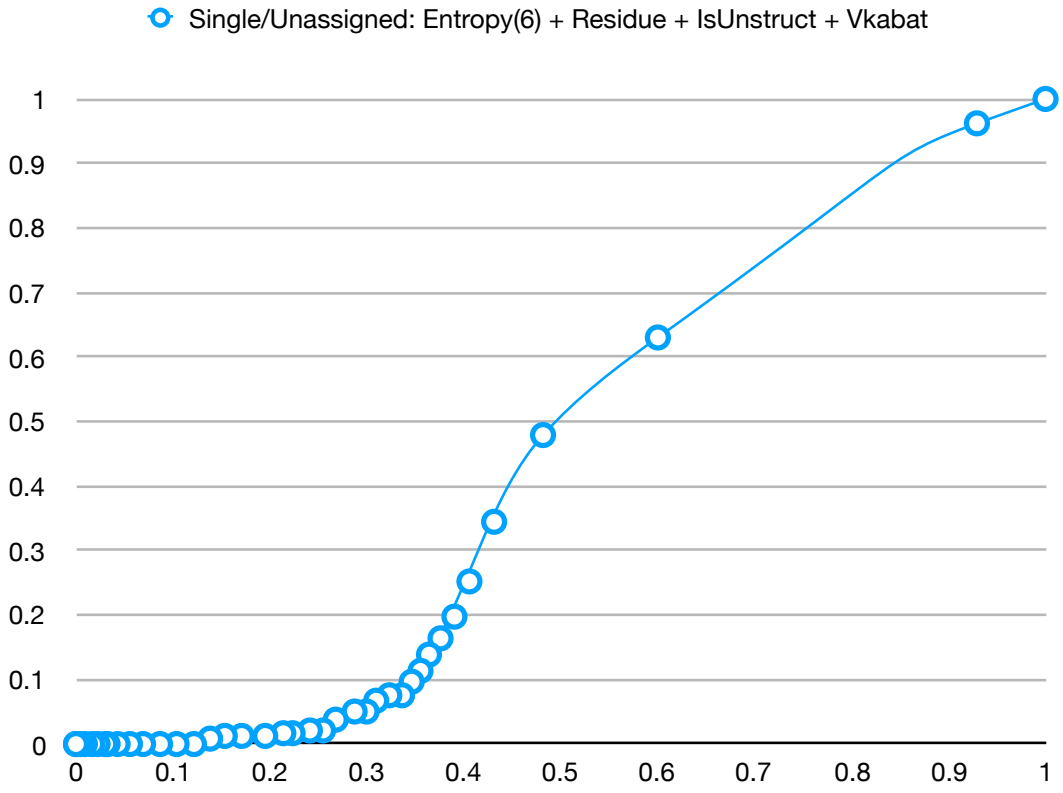
0.9
1


Single/Unassigned: Entropy(6) + Residue + IsUnstruct + Vkabat
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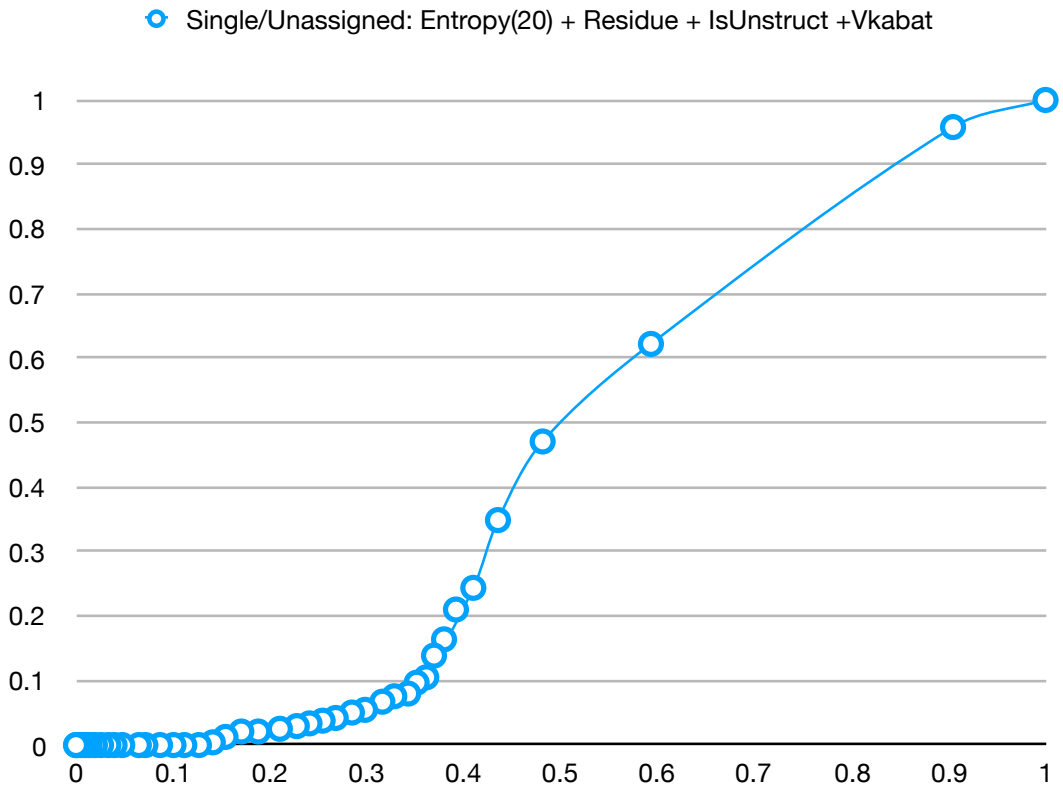
Single/Unassigned: Entropy(20) + Residue + IsUnstruct +Vkabat
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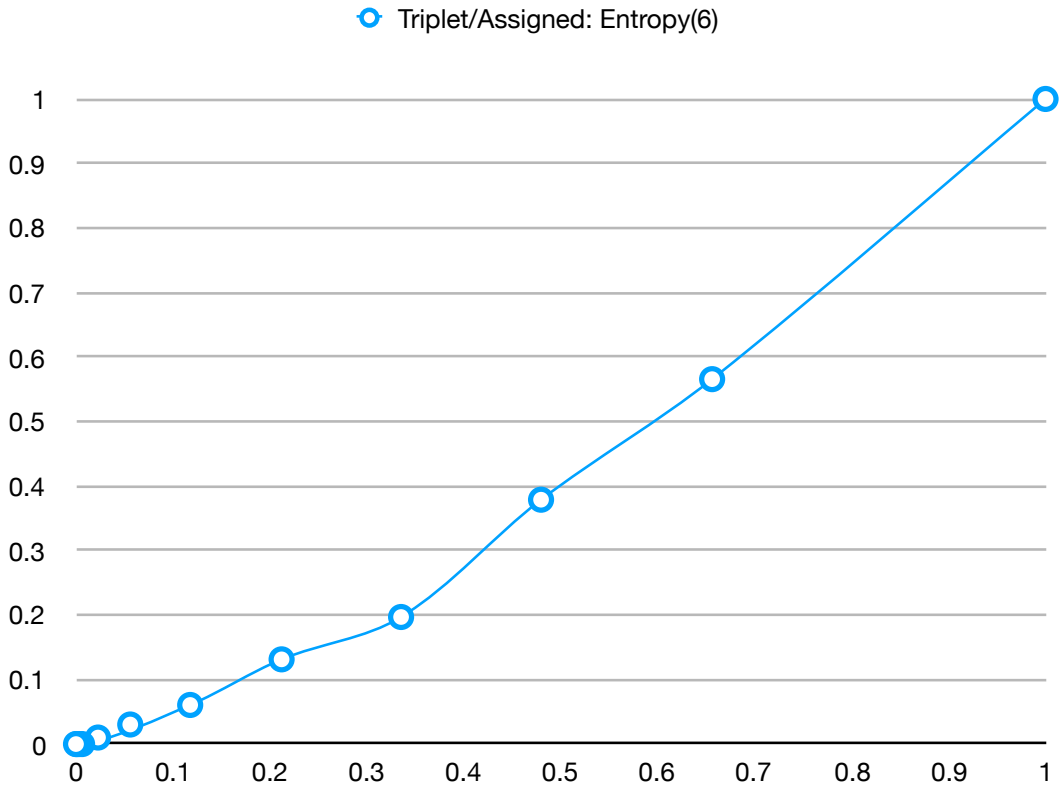
1


Triplet/Assigned: Entropy(6)
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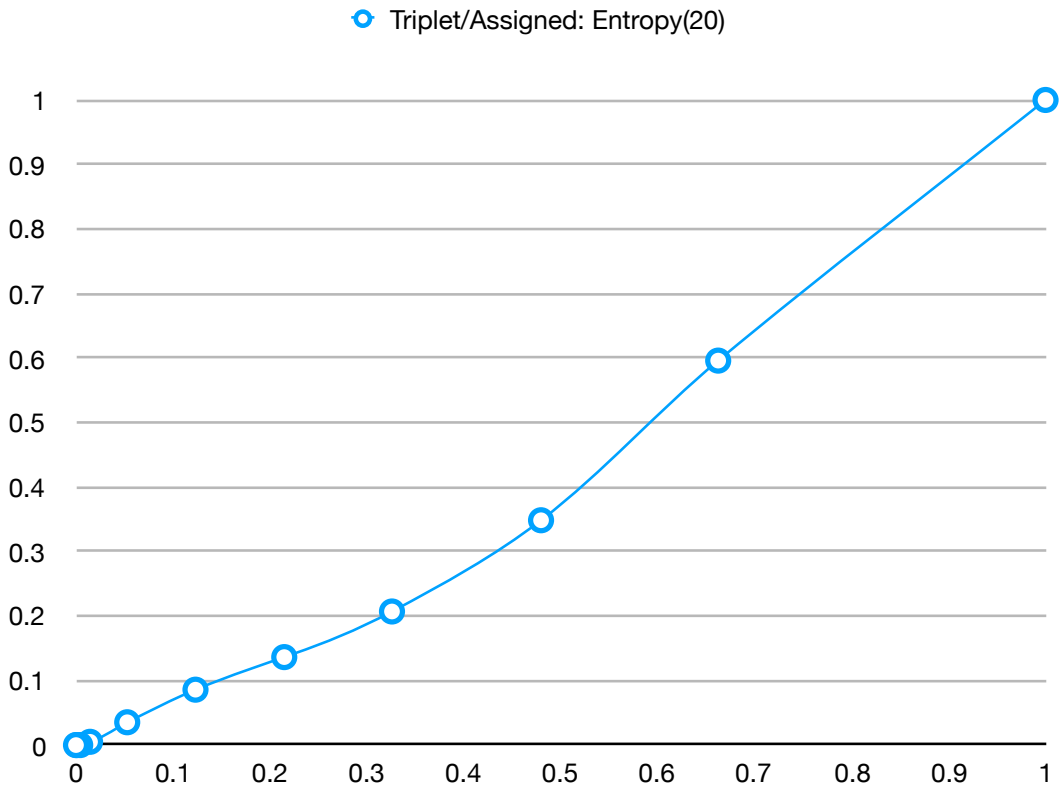
1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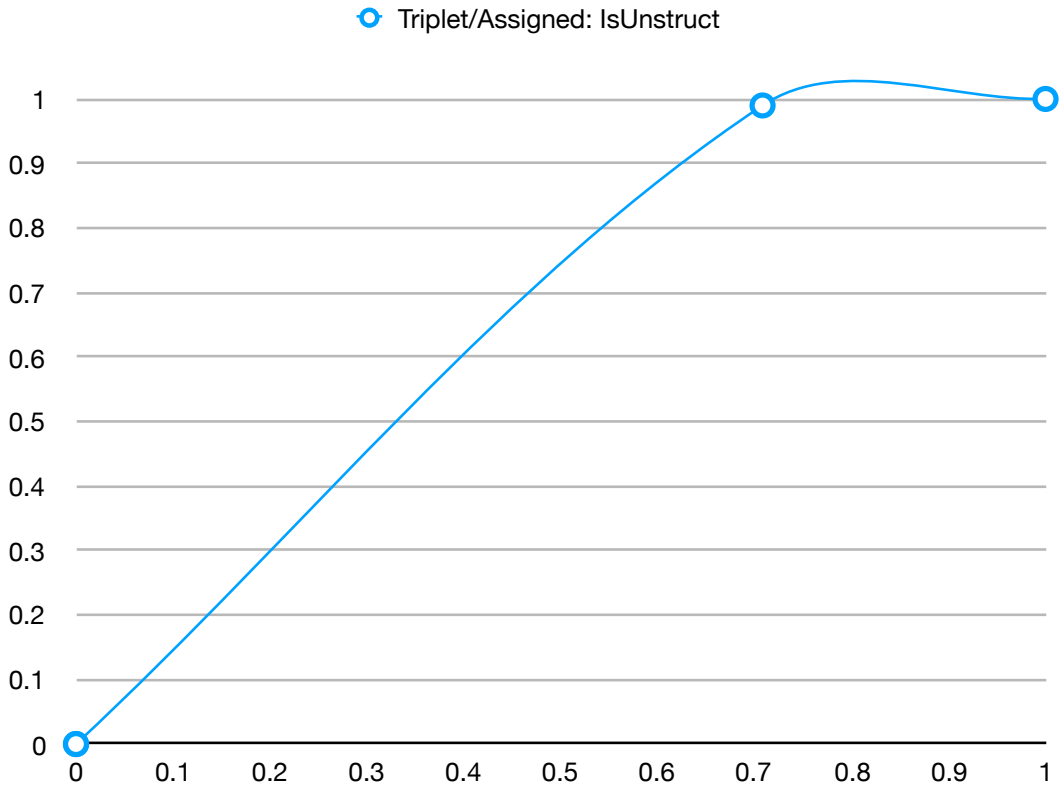
Triplet/Assigned: IsUnstruct
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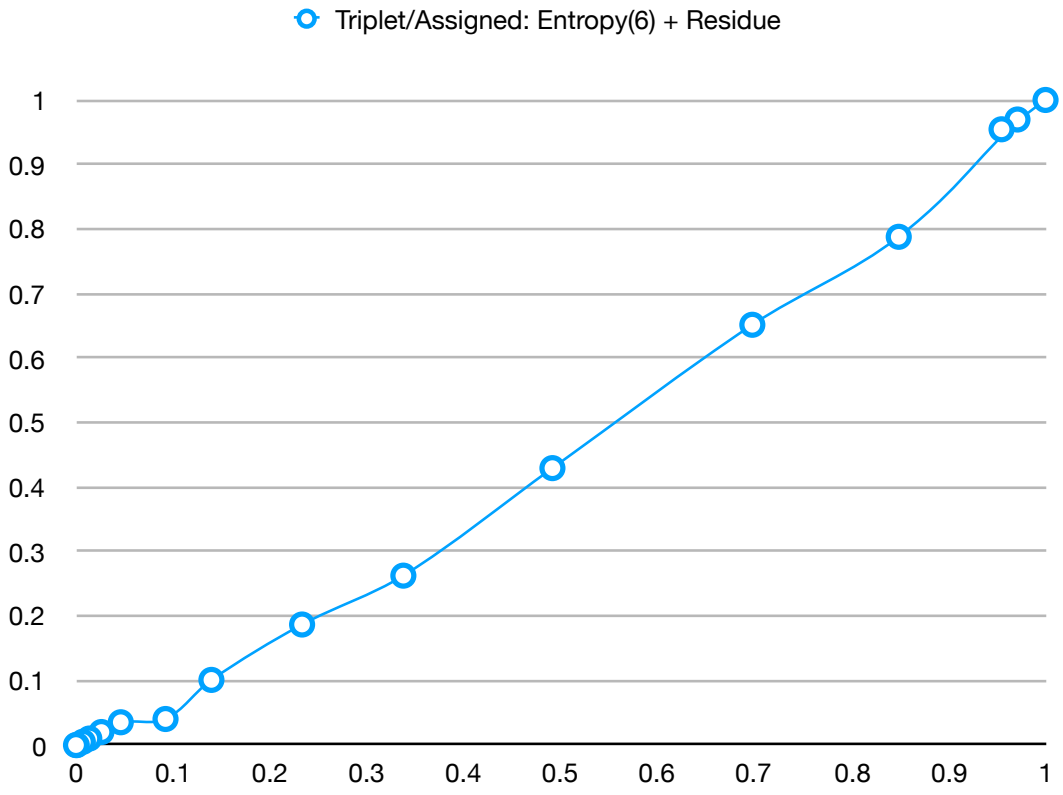
Triplet/Assigned: Entropy(6) + Residue
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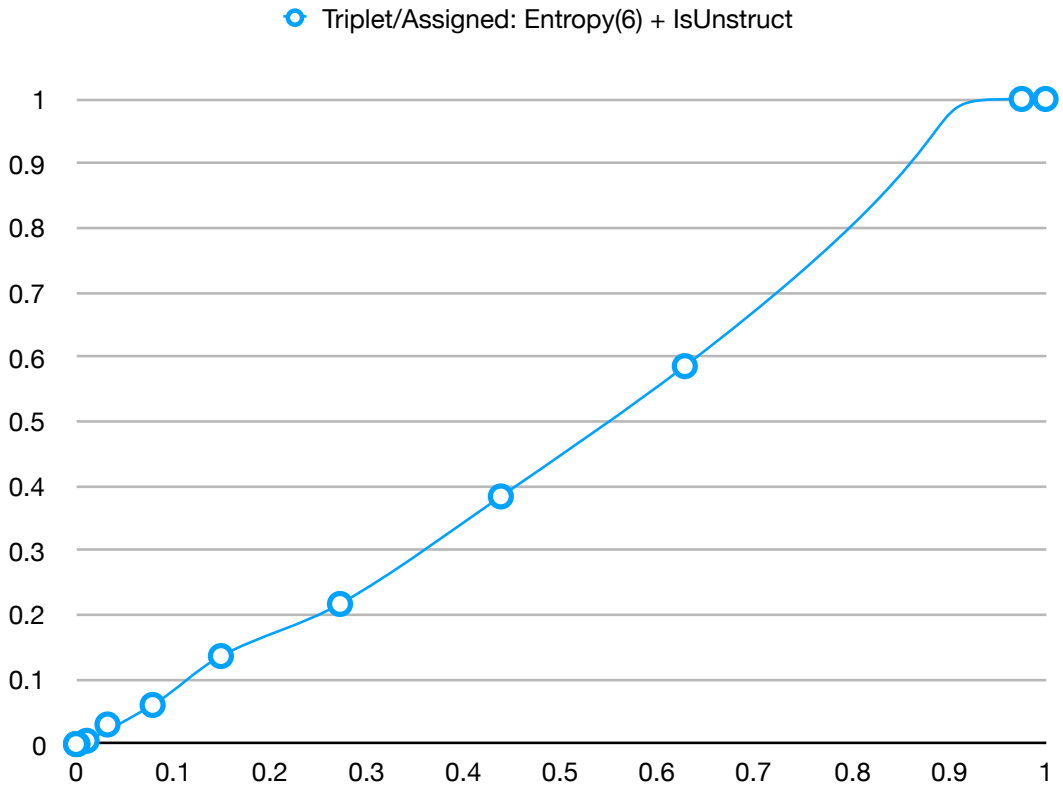
Triplet/Assigned: Entropy(6) + IsUnstruct
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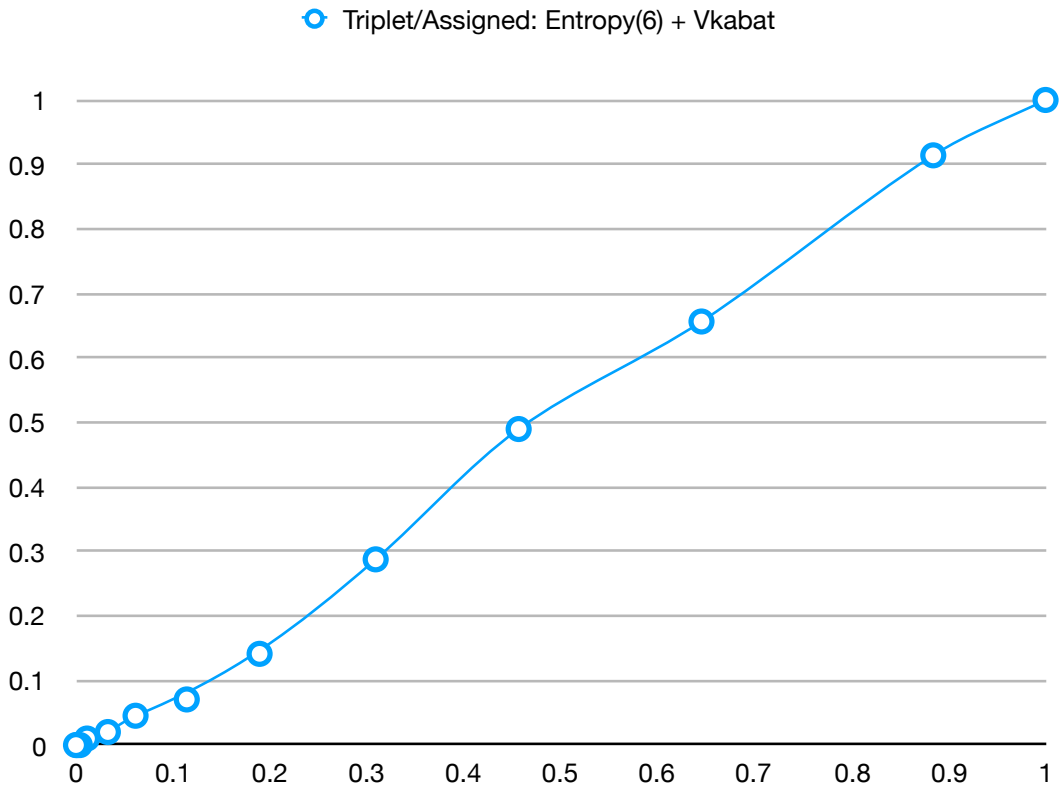
Triplet/Assigned: Entropy(6) + Vkabat
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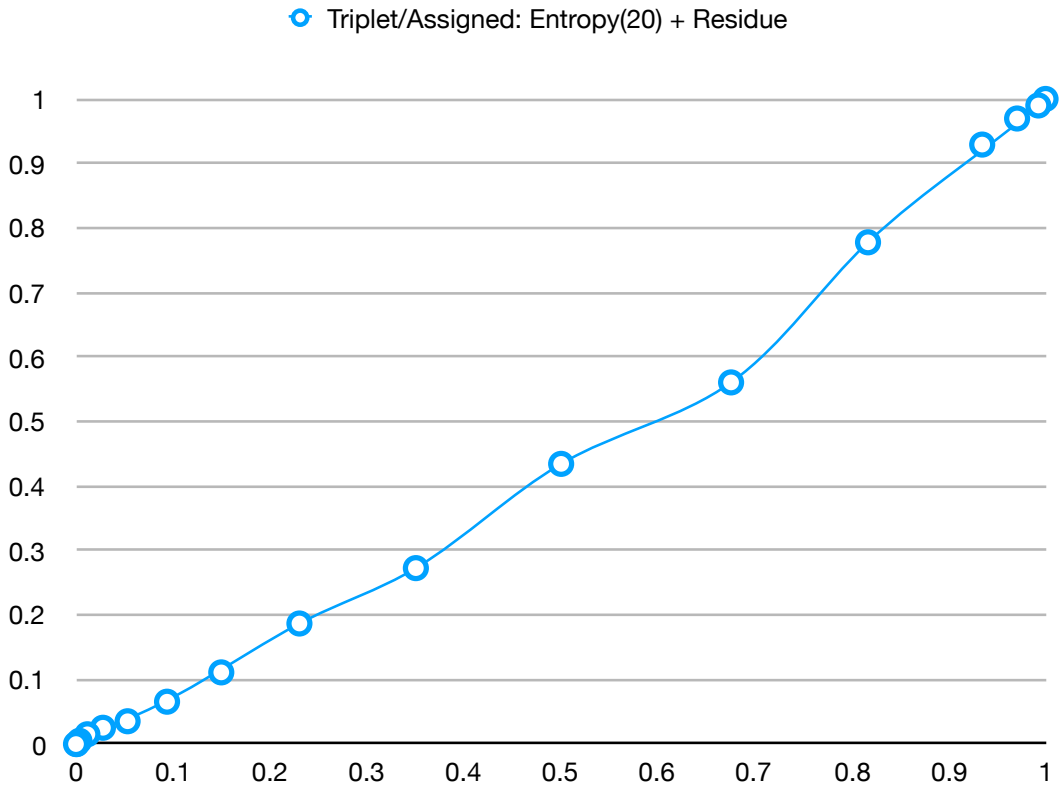
Triplet/Assigned: Entropy(20) + Residue
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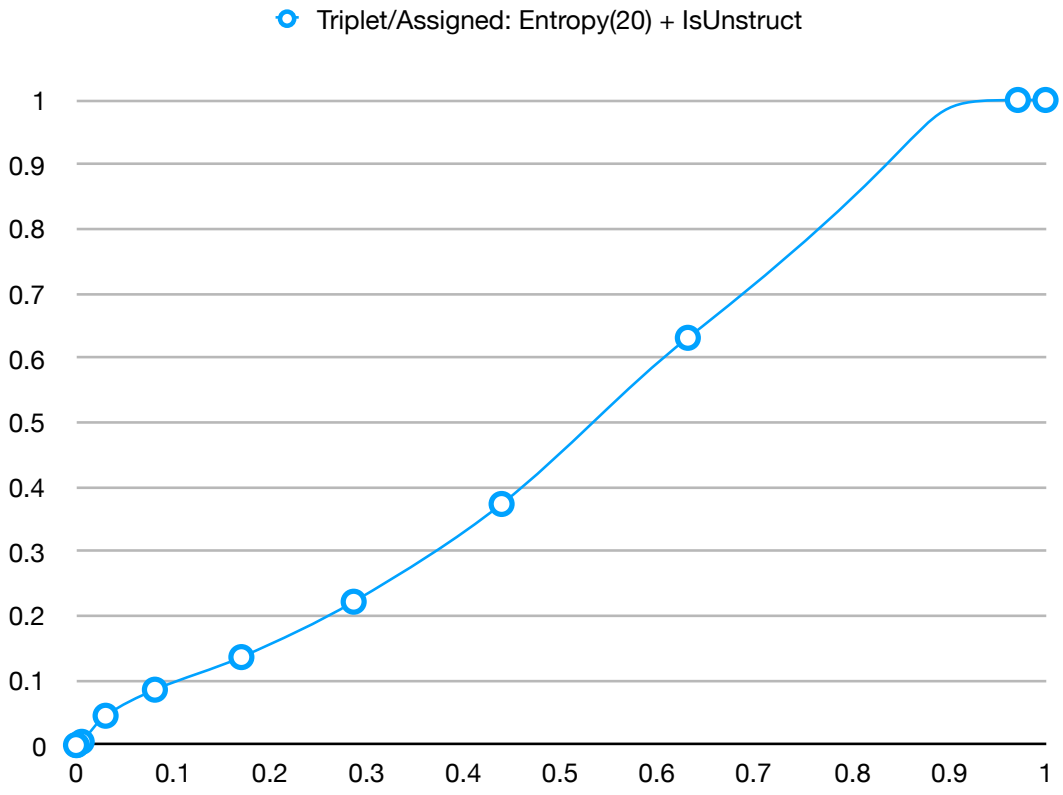
Triplet/Assigned: Entropy(20) + IsUnstruct
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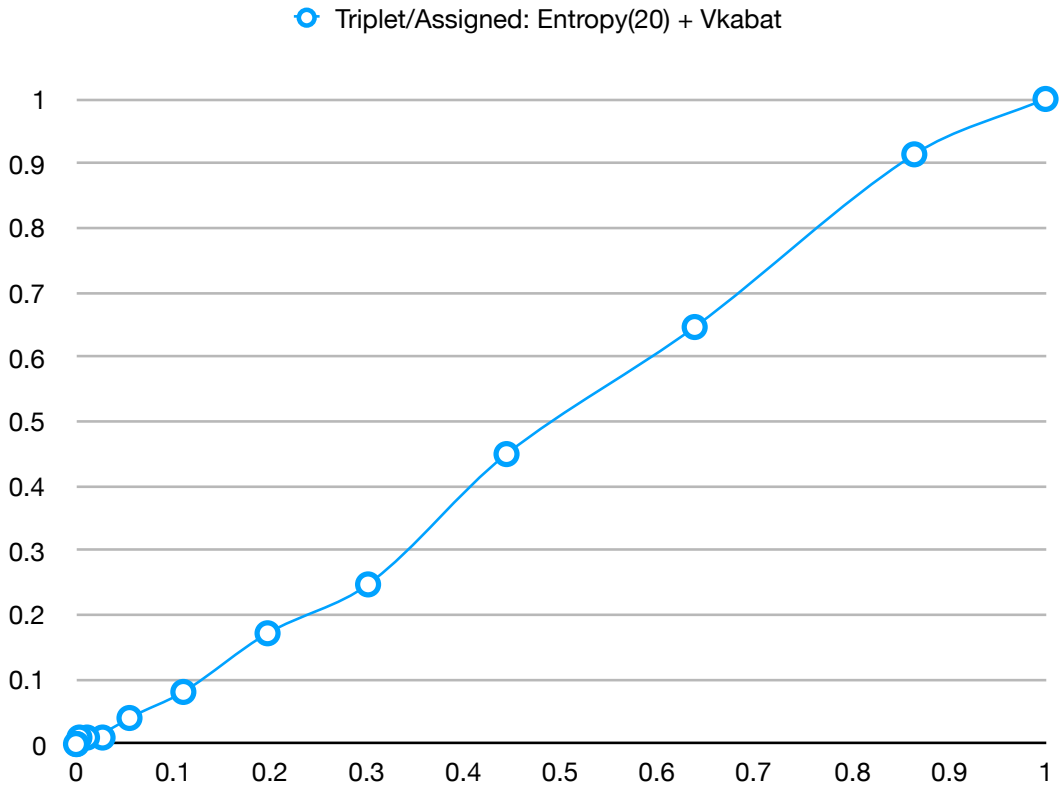
Triplet/Assigned: Entropy(20) + Vkabat
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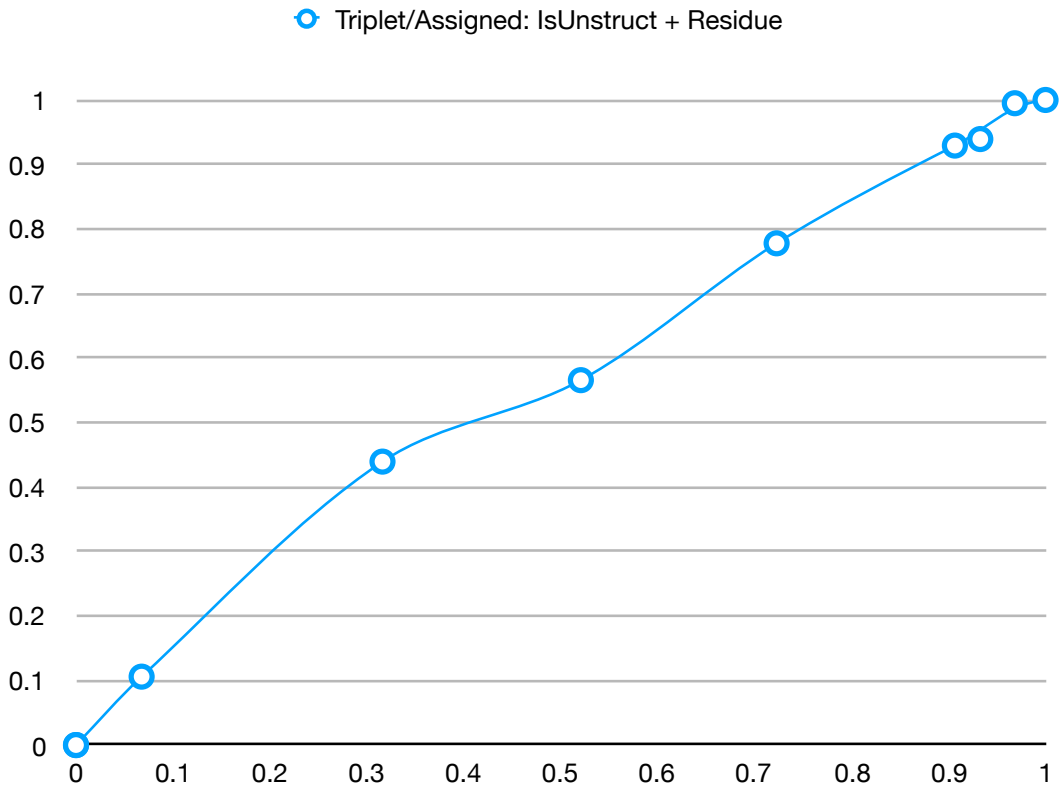
Triplet/Assigned: IsUnstruct + Residue
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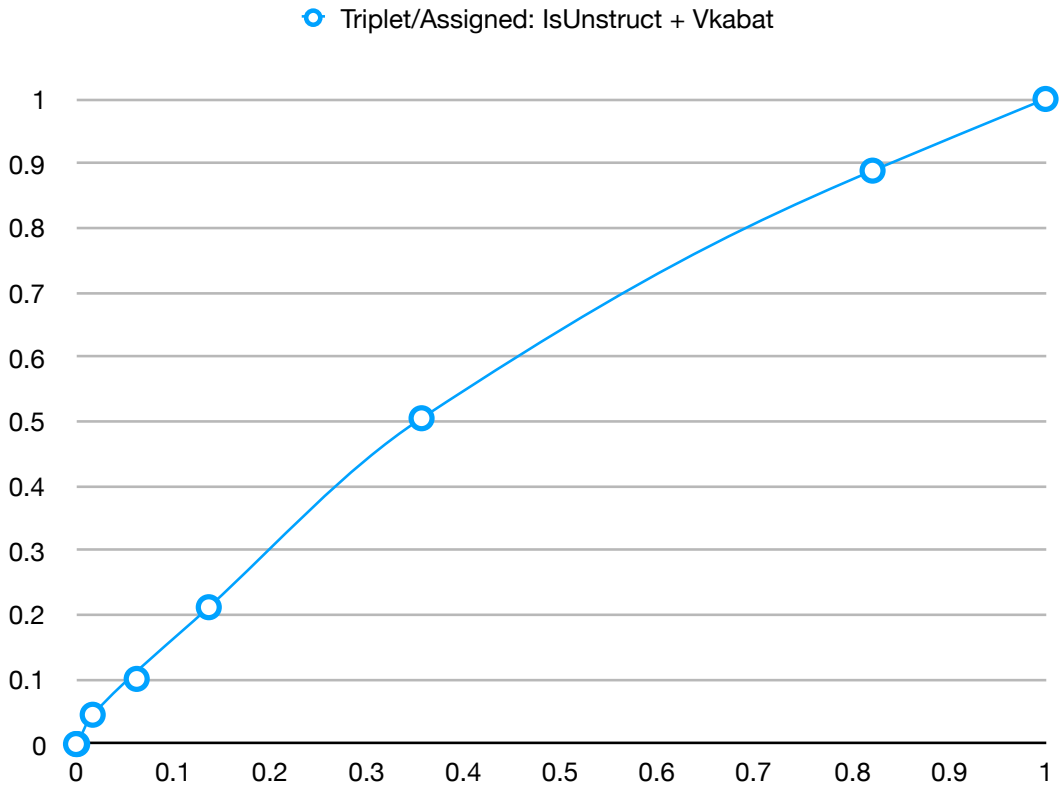
Triplet/Assigned: IsUnstruct + Vkabat
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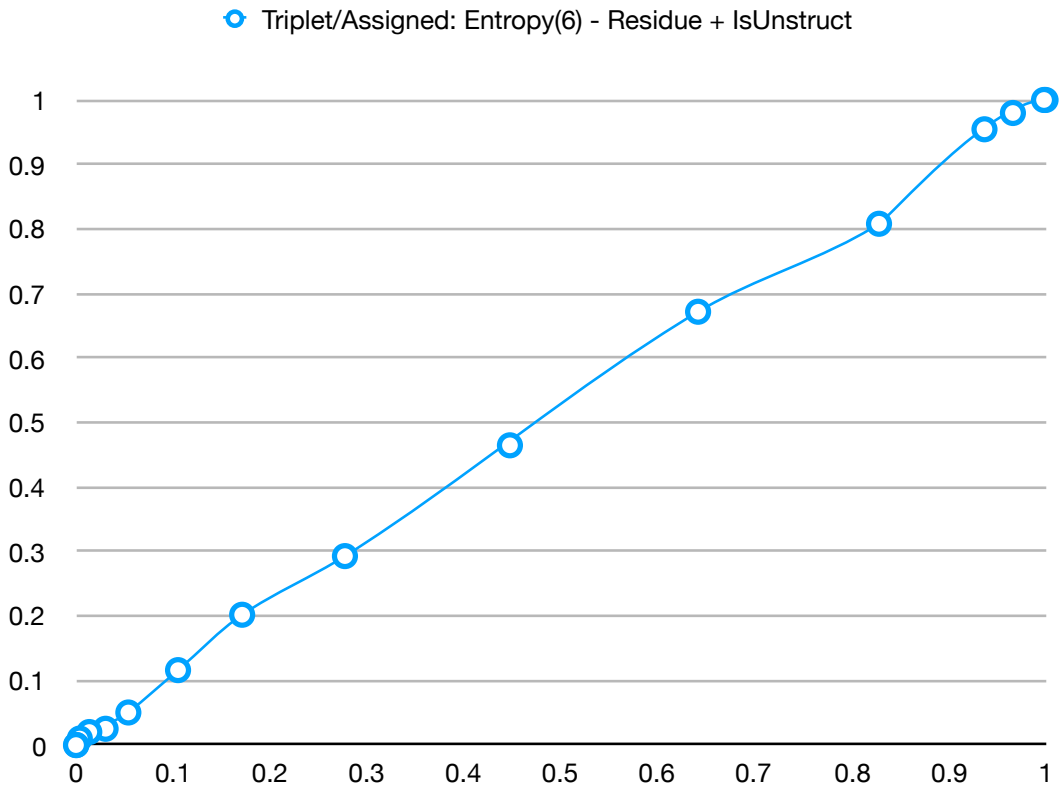
Triplet/Assigned: Entropy(6) - Residue + IsUnstruct
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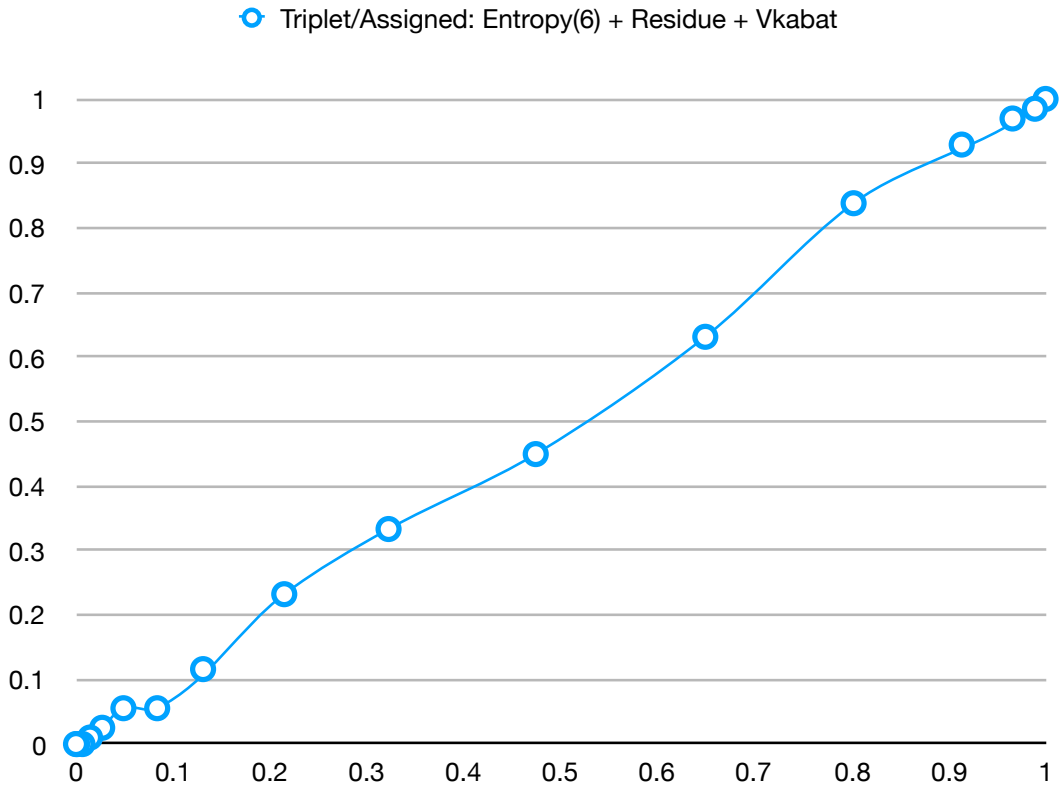
Triplet/Assigned: Entropy(6) + Residue + Vkabat
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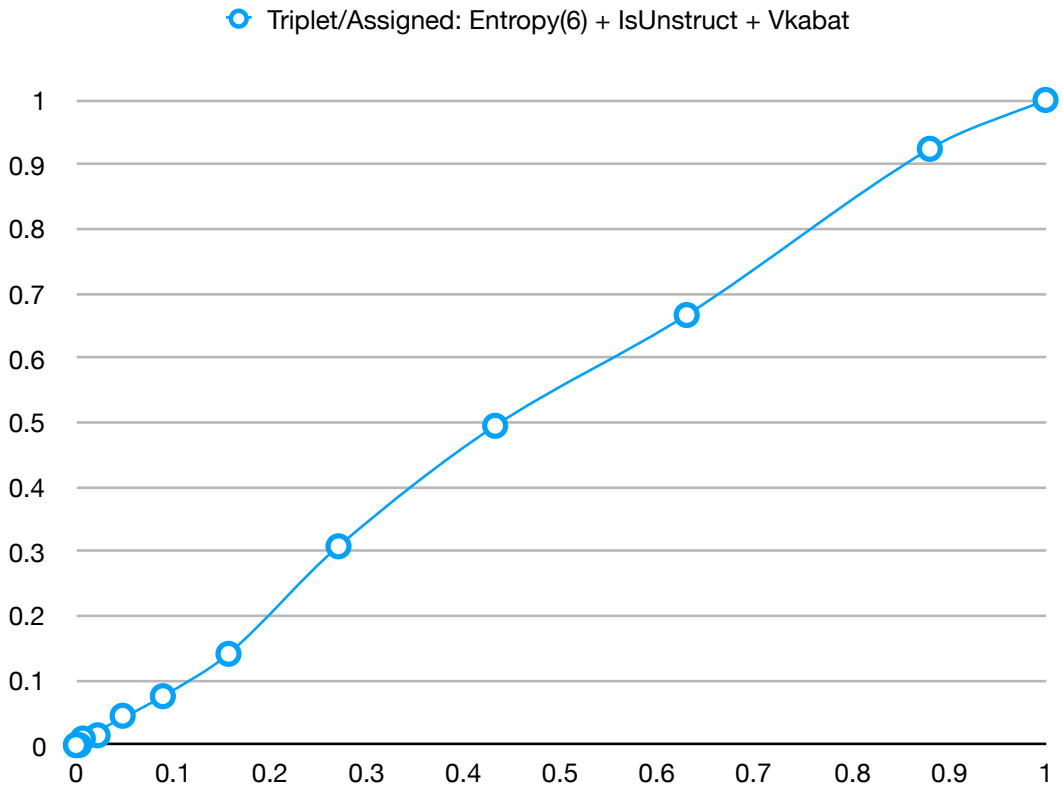
Triplet/Assigned: Entropy(6) + IsUnstruct + Vkabat
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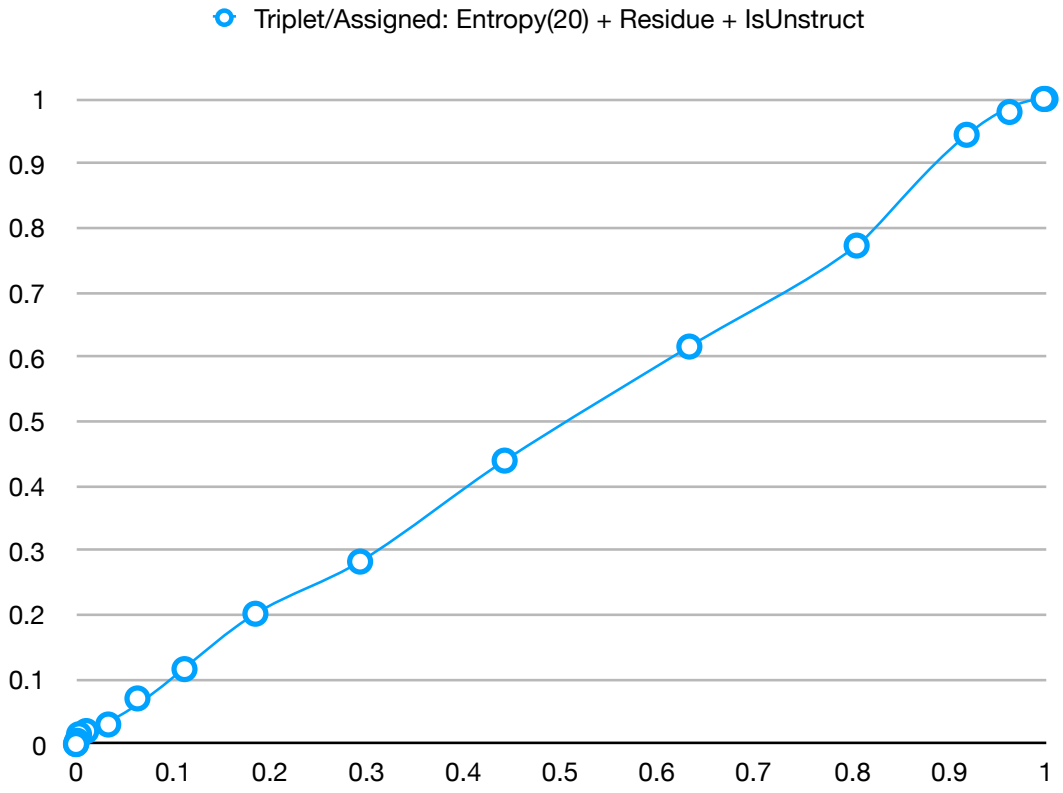
Triplet/Assigned: Entropy(20) + Residue + IsUnstruct
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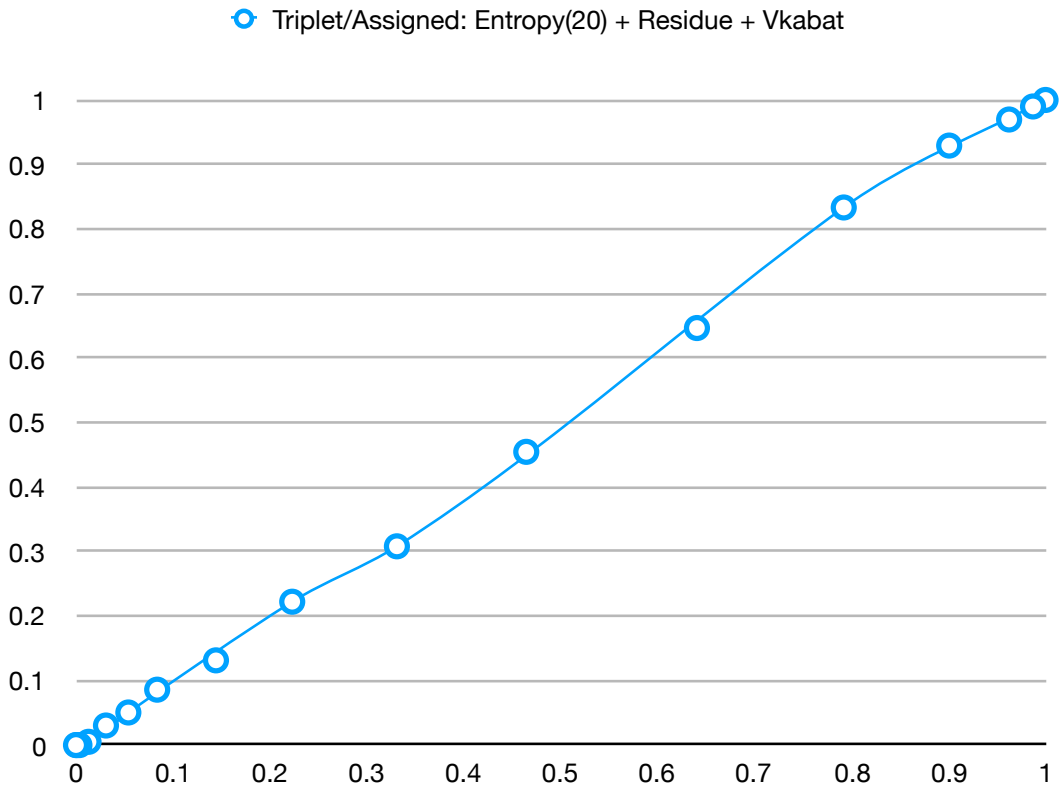
Triplet/Assigned: Entropy(20) + Residue + Vkabat
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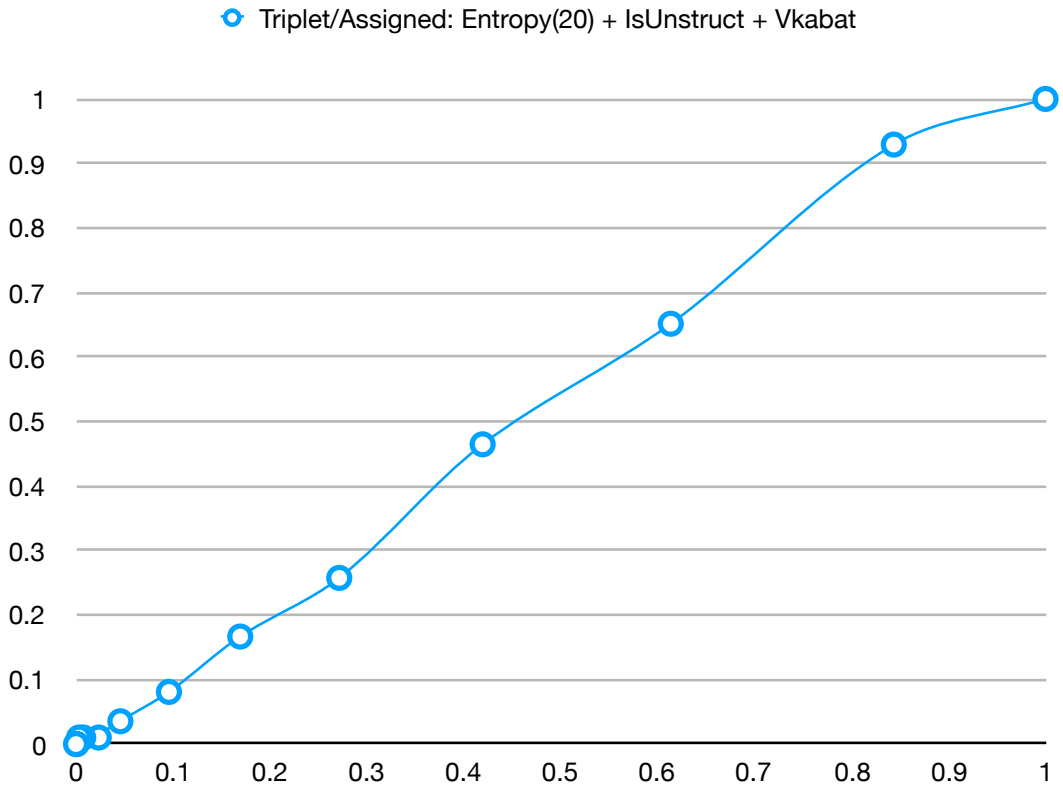
Triplet/Assigned: Entropy(20) + IsUnstruct + Vkabat
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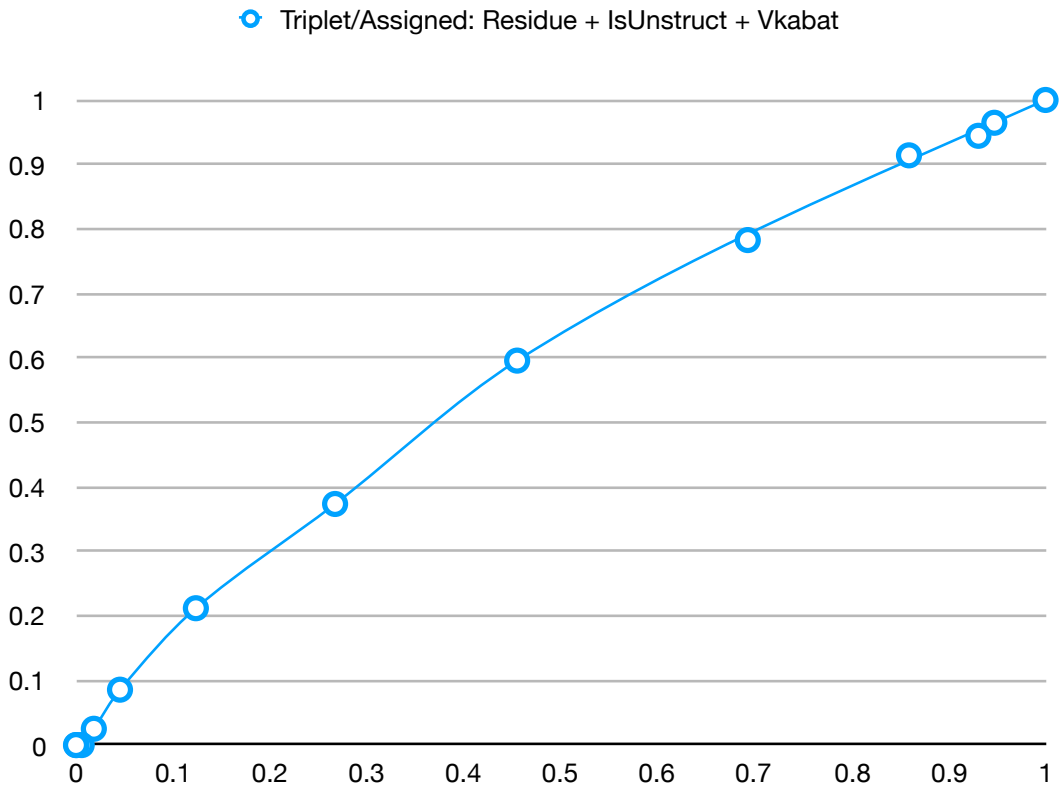
Triplet/Assigned: Residue + IsUnstruct + Vkabat
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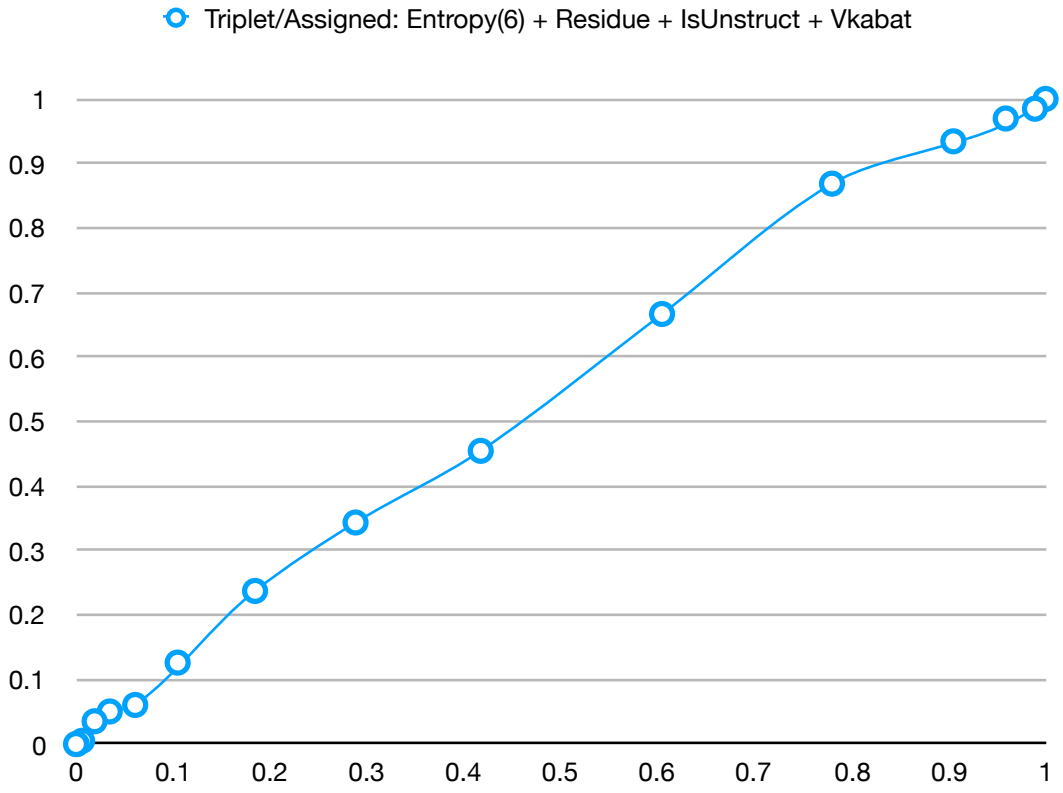
Triplet/Assigned: Entropy(6) + Residue + IsUnstruct + Vkabat
1
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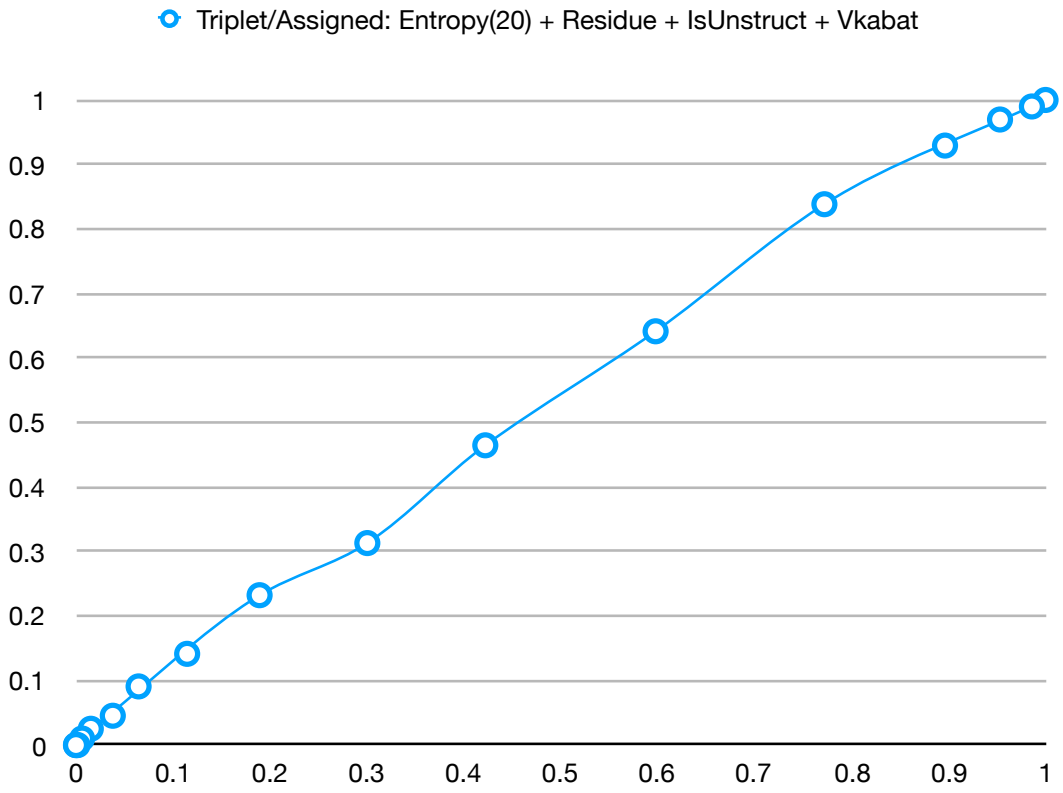
Triplet/Assigned: Entropy(20) + Residue + IsUnstruct + Vkabat
1
0.9
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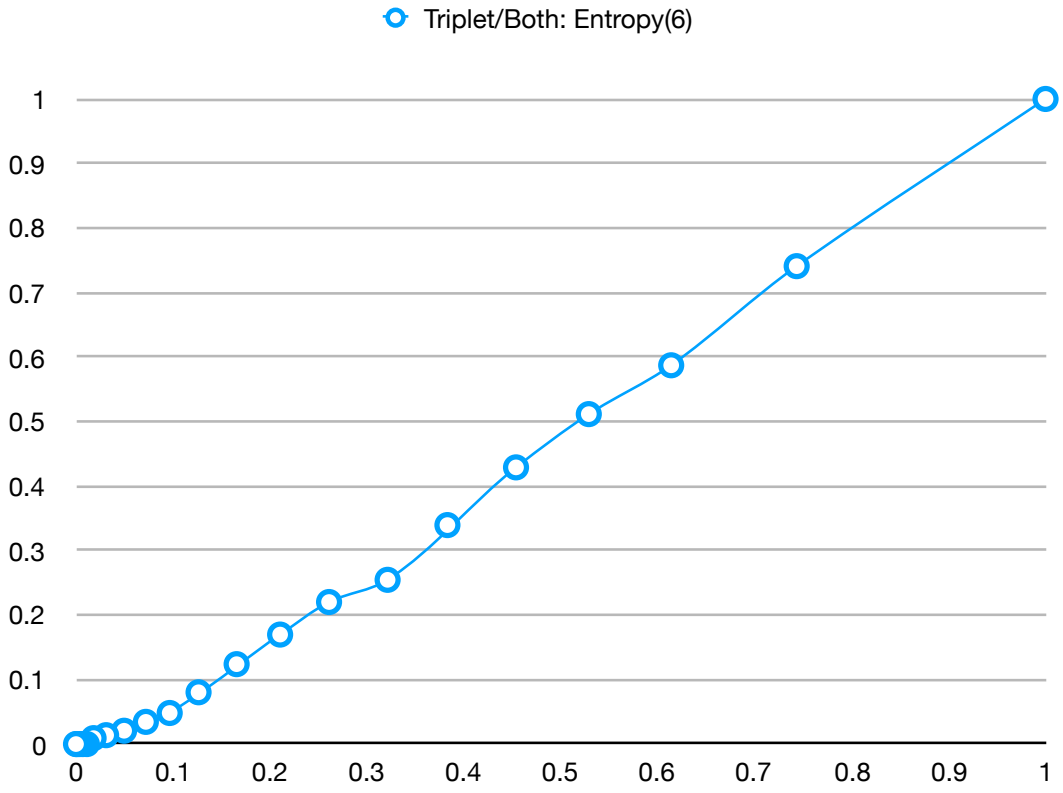
Triplet/Both: Entropy(6)
1
0.9
0.8
0.7
0.6
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0.4
0.3
0.2
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0.1
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0.4
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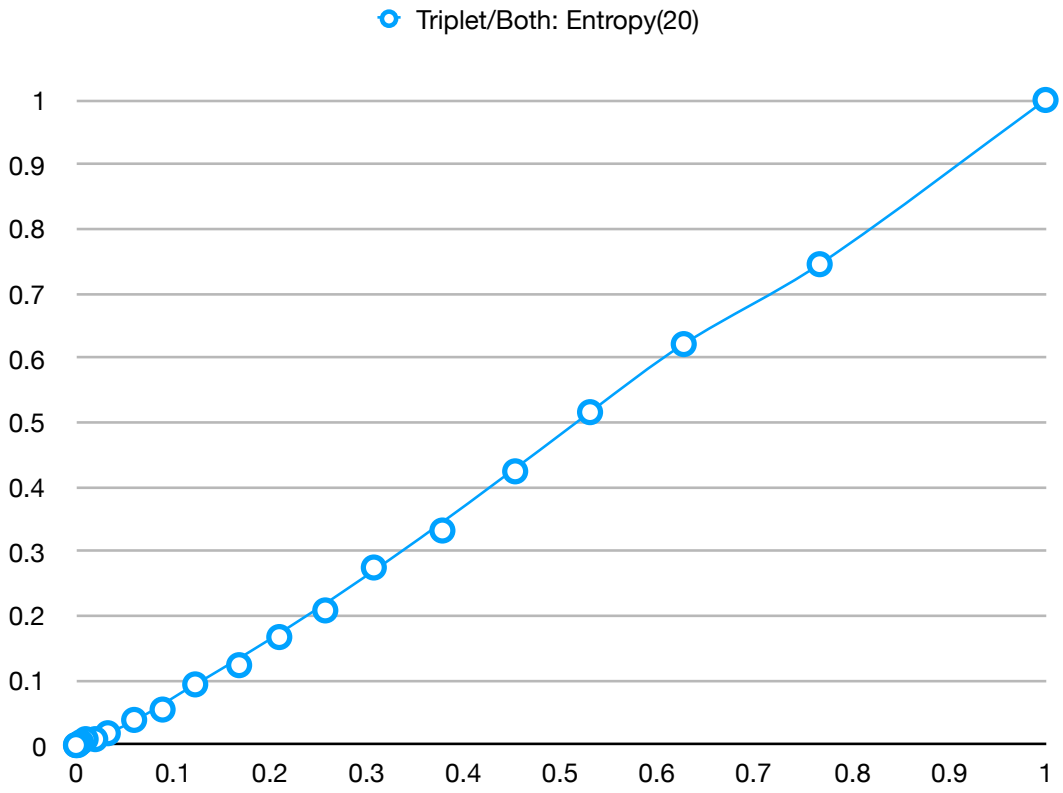
0.9
1


Triplet/Both: Entropy(20)
1
0.9
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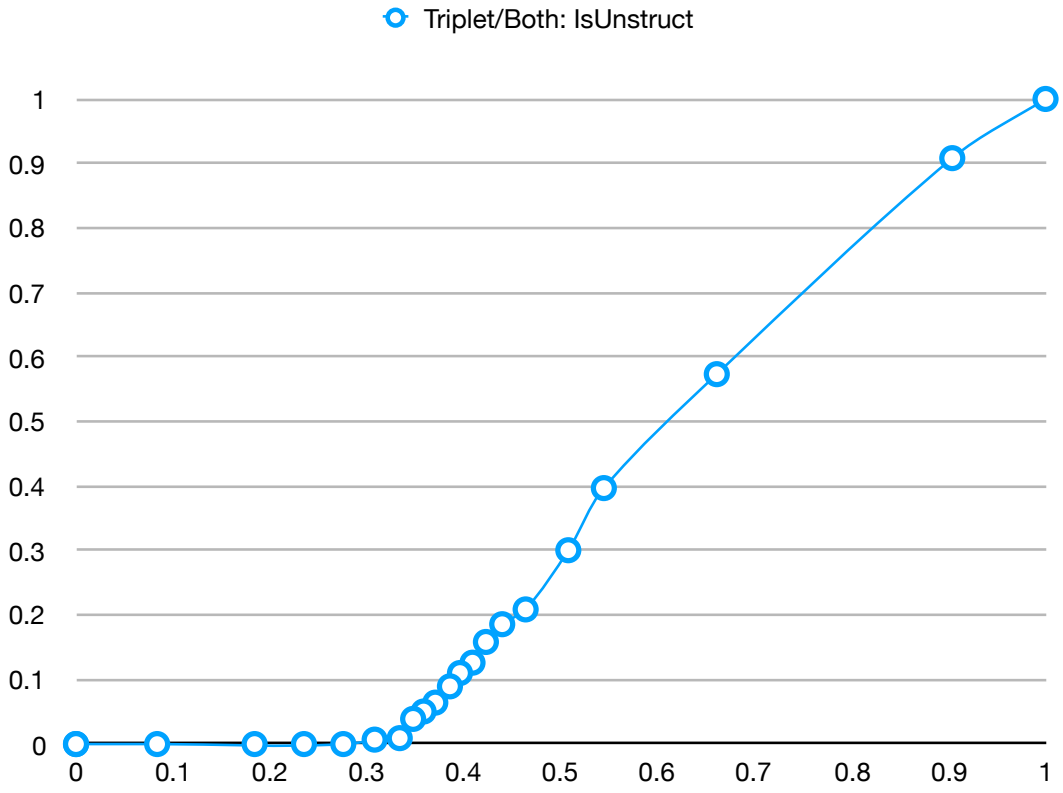
Triplet/Both: IsUnstruct
1
0.9
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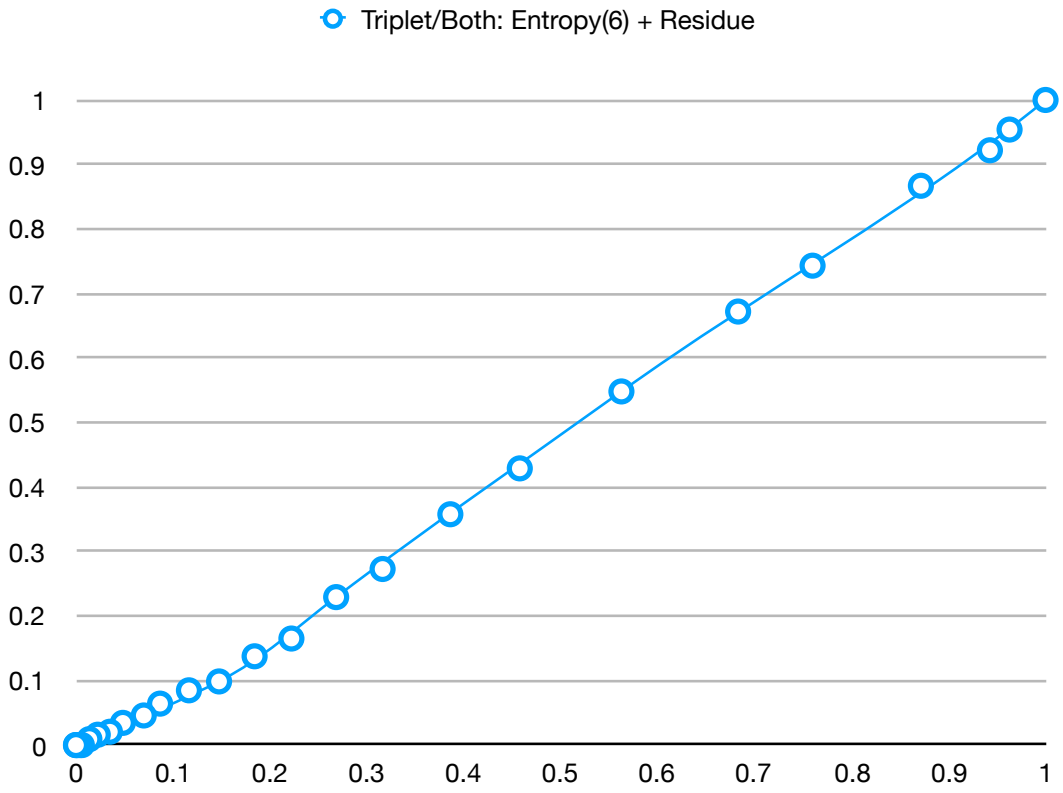
0.9
1


Triplet/Both: Entropy(6) + Residue
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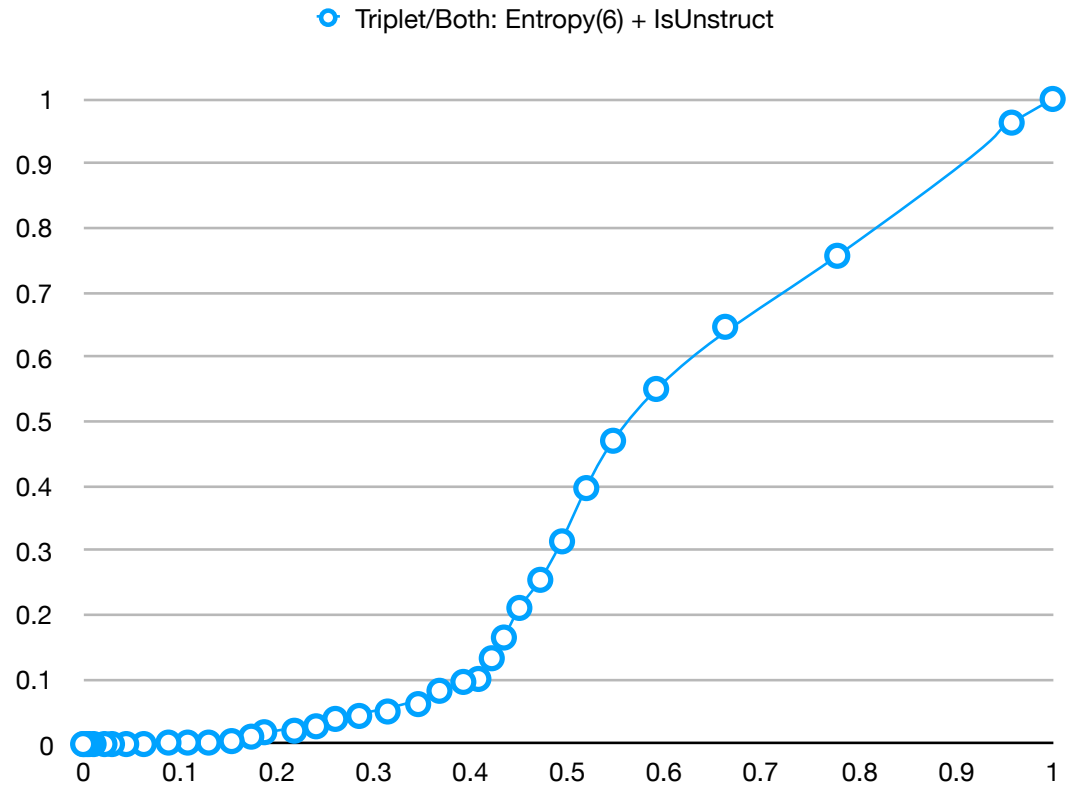
1


Triplet/Both: Entropy(6) + IsUnstruct
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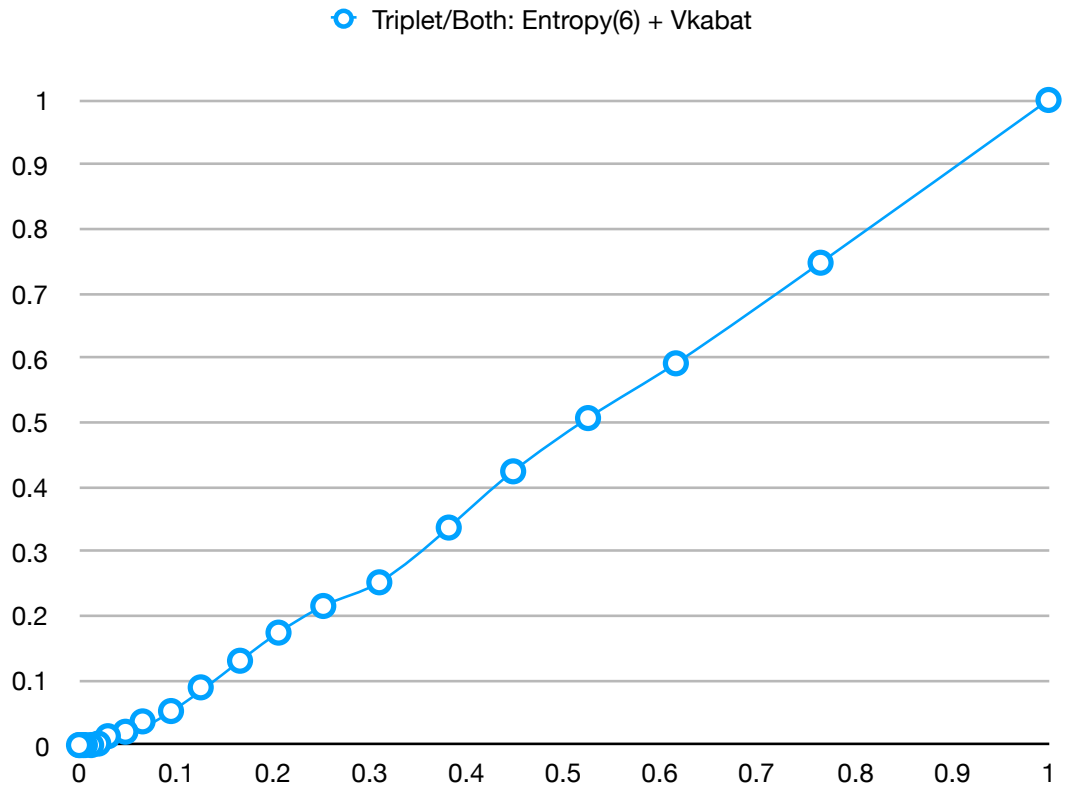
Triplet/Both: Entropy(6) + Vkabat
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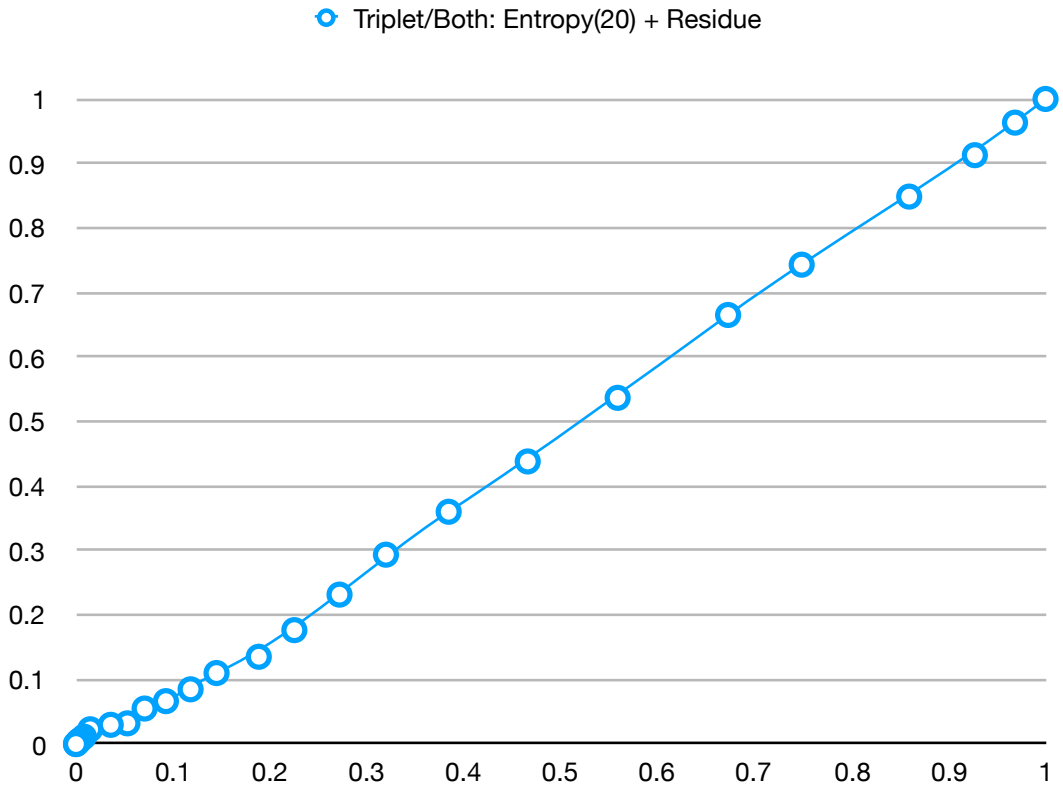
0.9
1


Triplet/Both: Entropy(20) + Residue
1
0.9
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0.9
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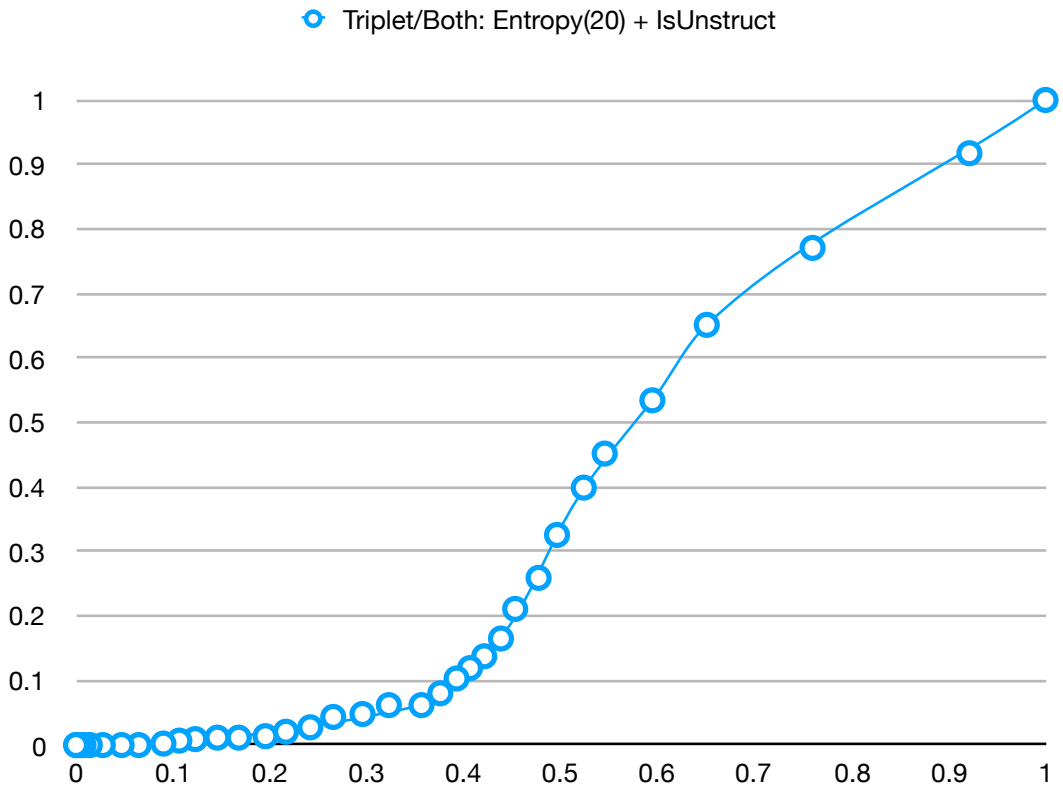
Triplet/Both: Entropy(20) + IsUnstruct
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0.9
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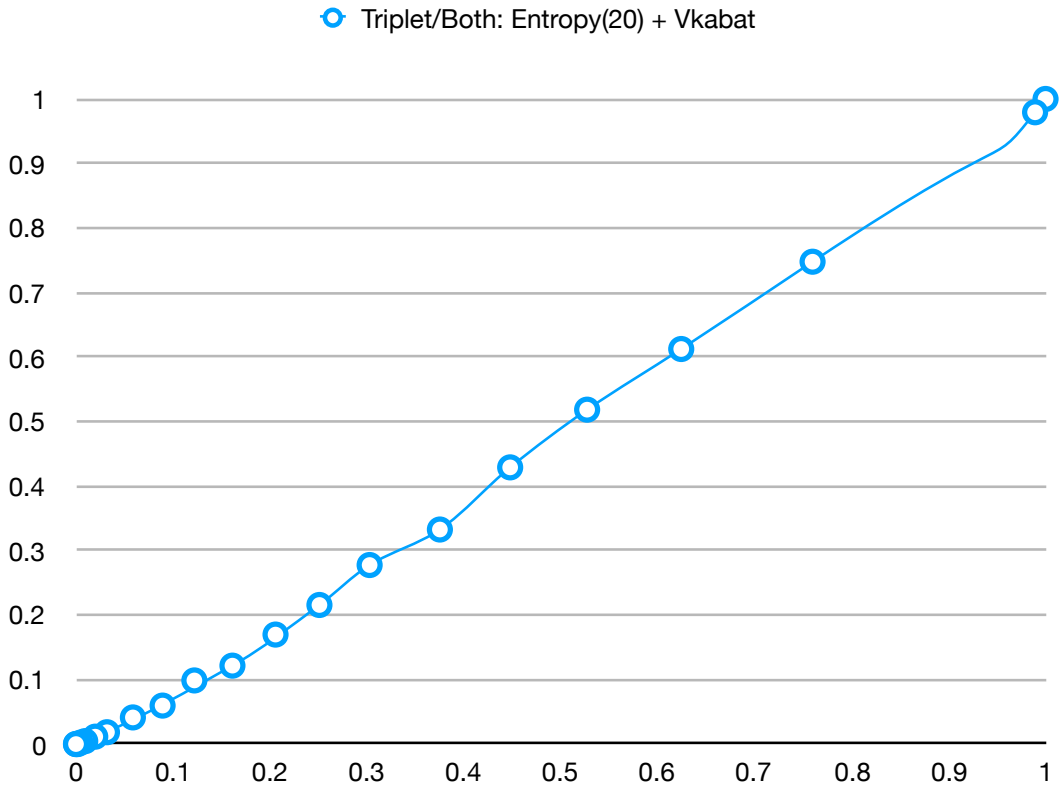
Triplet/Both: Entropy(20) + Vkabat
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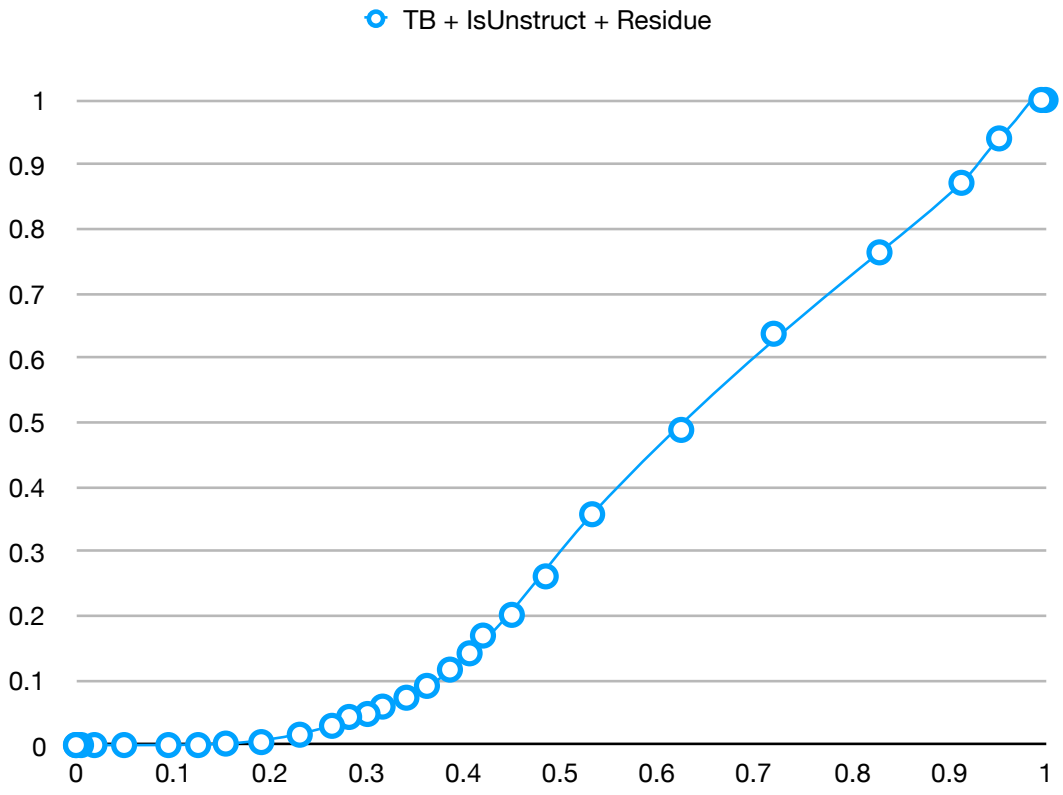
1


TB + IsUnstruct + Residue
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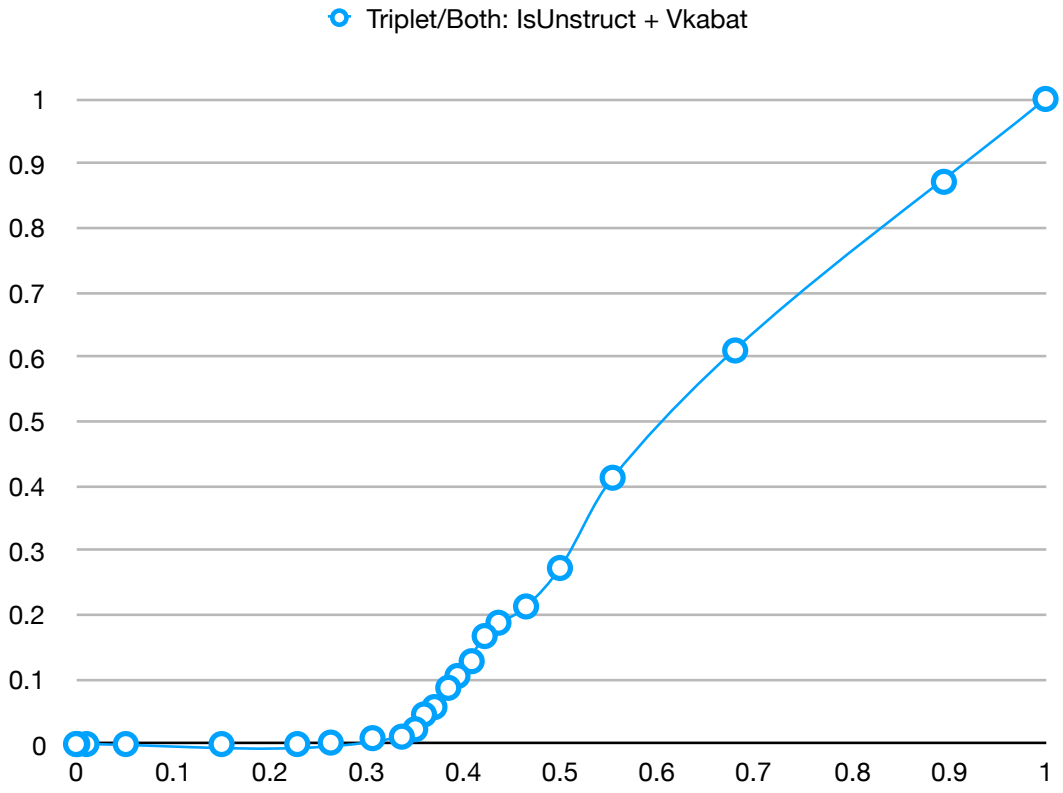
1


Triplet/Both: IsUnstruct + Vkabat
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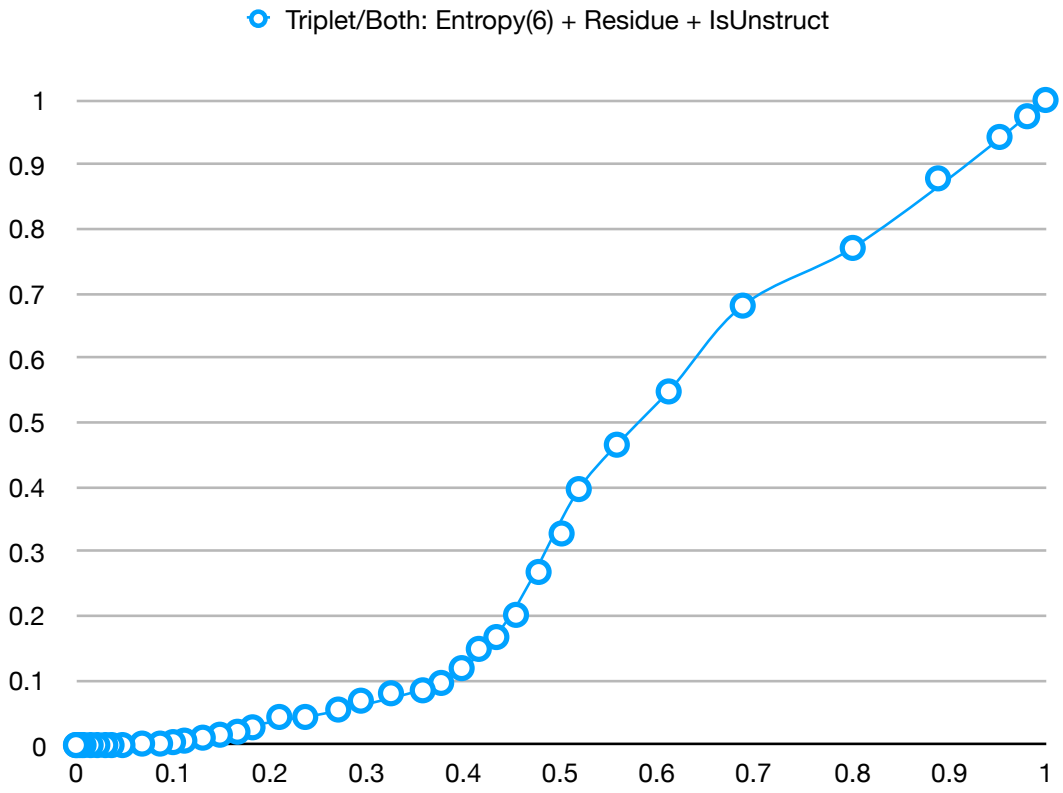
Triplet/Both: Entropy(6) + Residue + IsUnstruct
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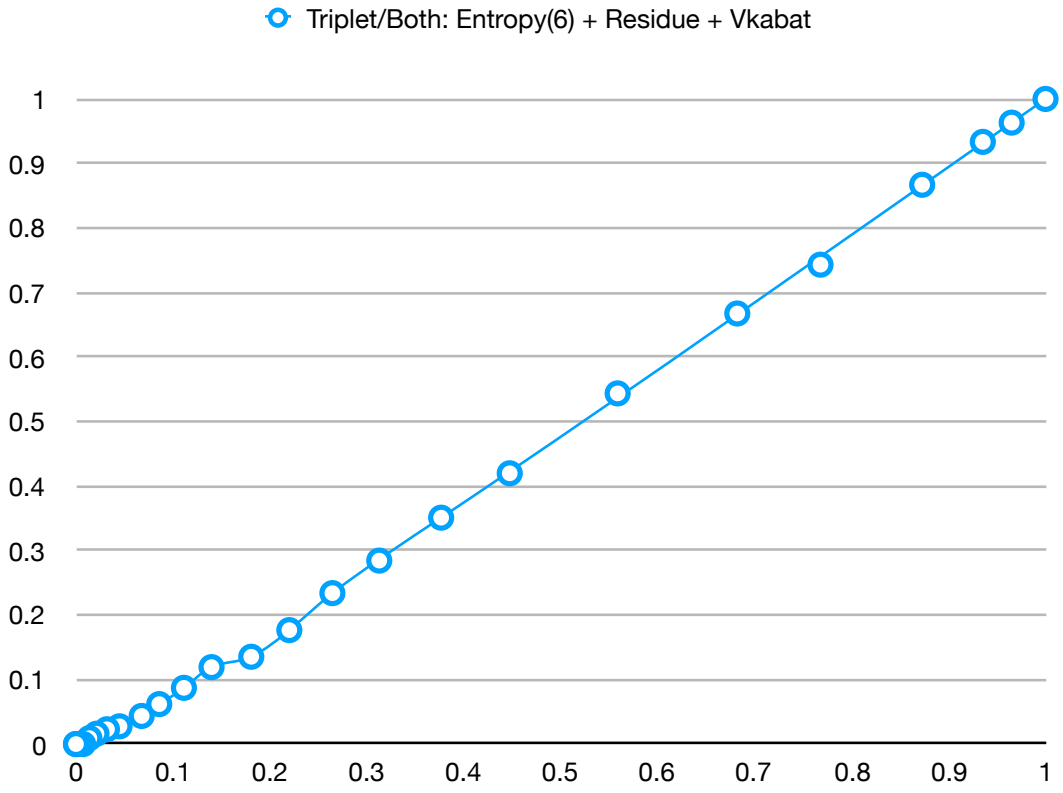
Triplet/Both: Entropy(6) + Residue + Vkabat
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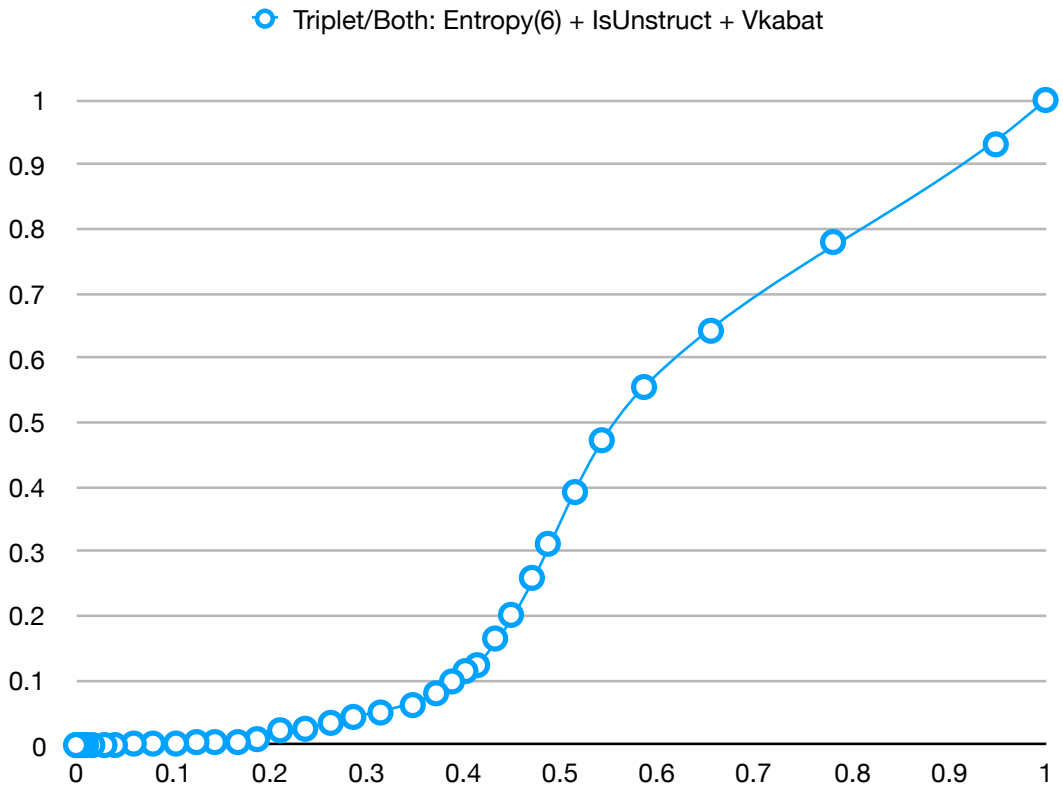
Triplet/Both: Entropy(6) + IsUnstruct + Vkabat
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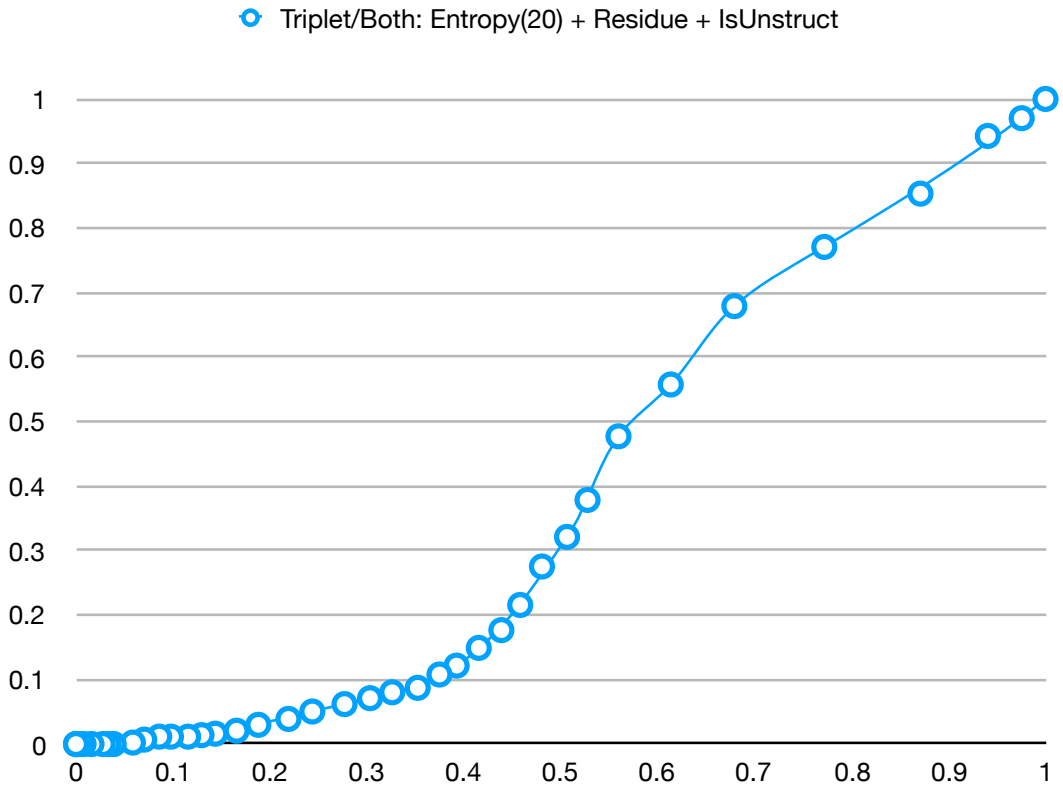
Triplet/Both: Entropy(20) + Residue + IsUnstruct
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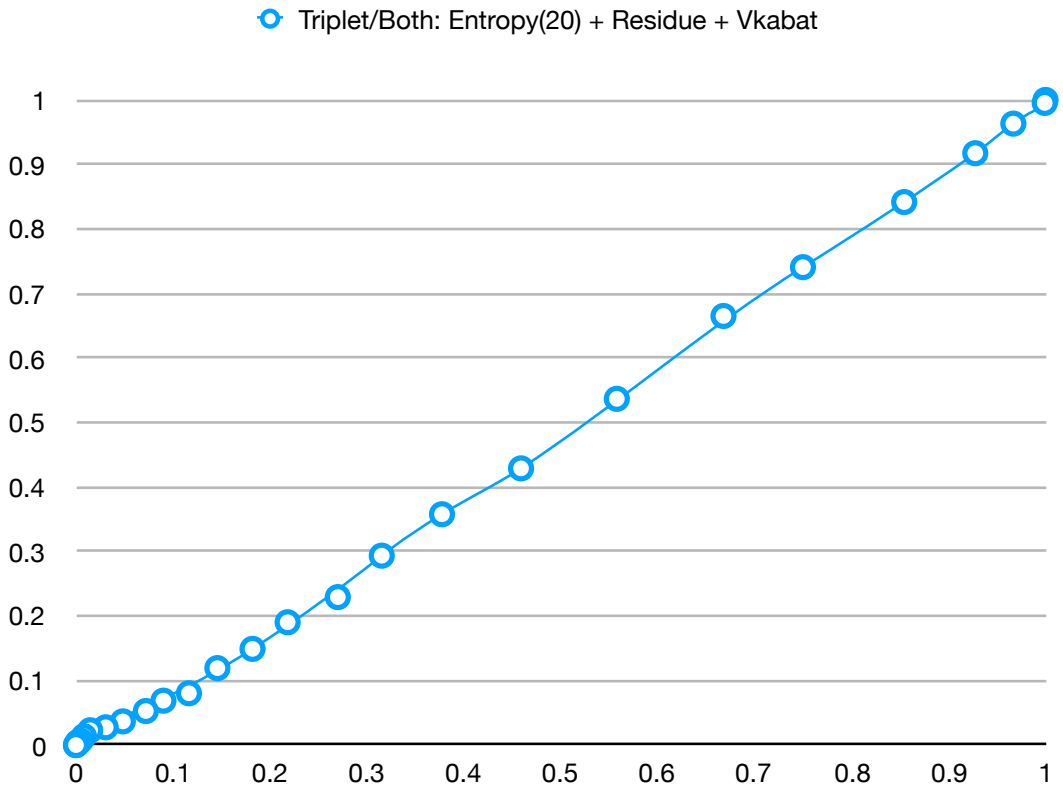
Triplet/Both: Entropy(20) + Residue + Vkabat
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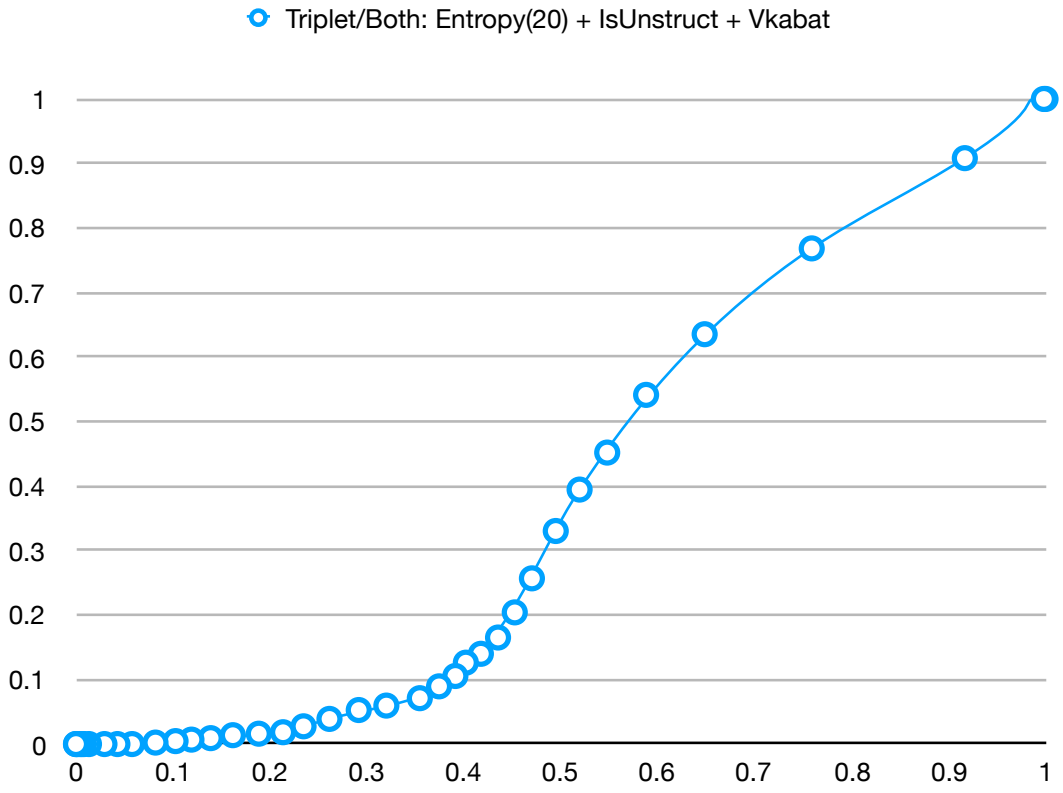
Triplet/Both: Entropy(20) + IsUnstruct + Vkabat
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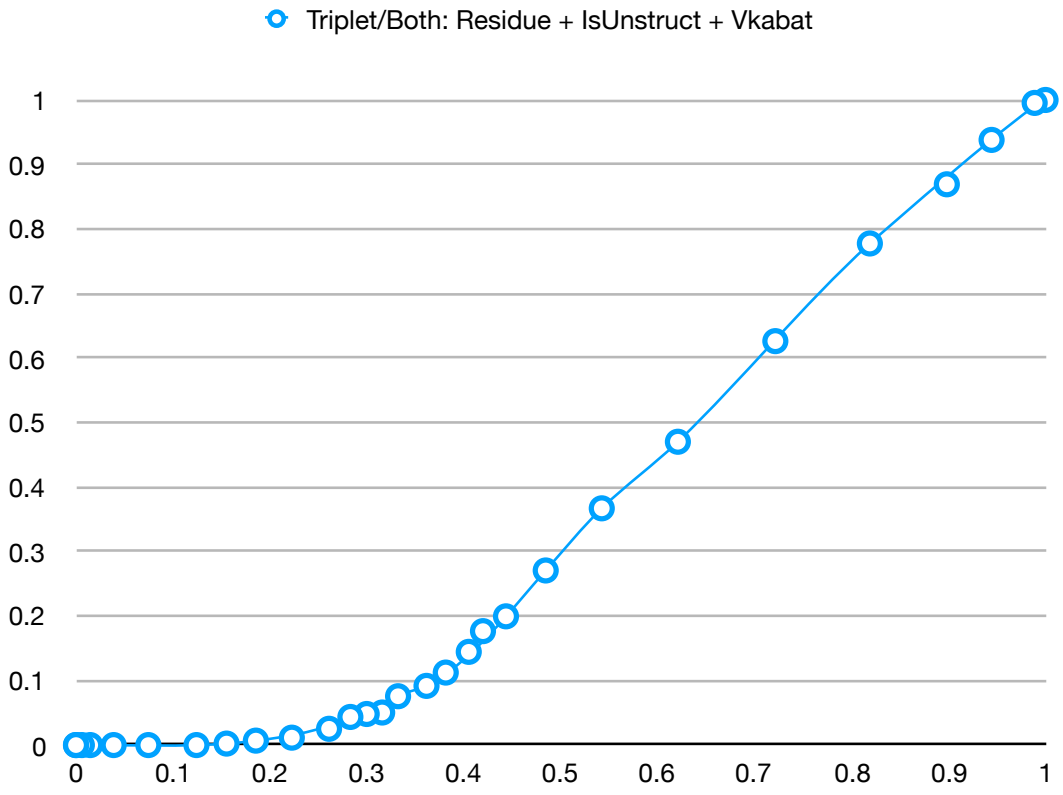
Triplet/Both: Residue + IsUnstruct + Vkabat
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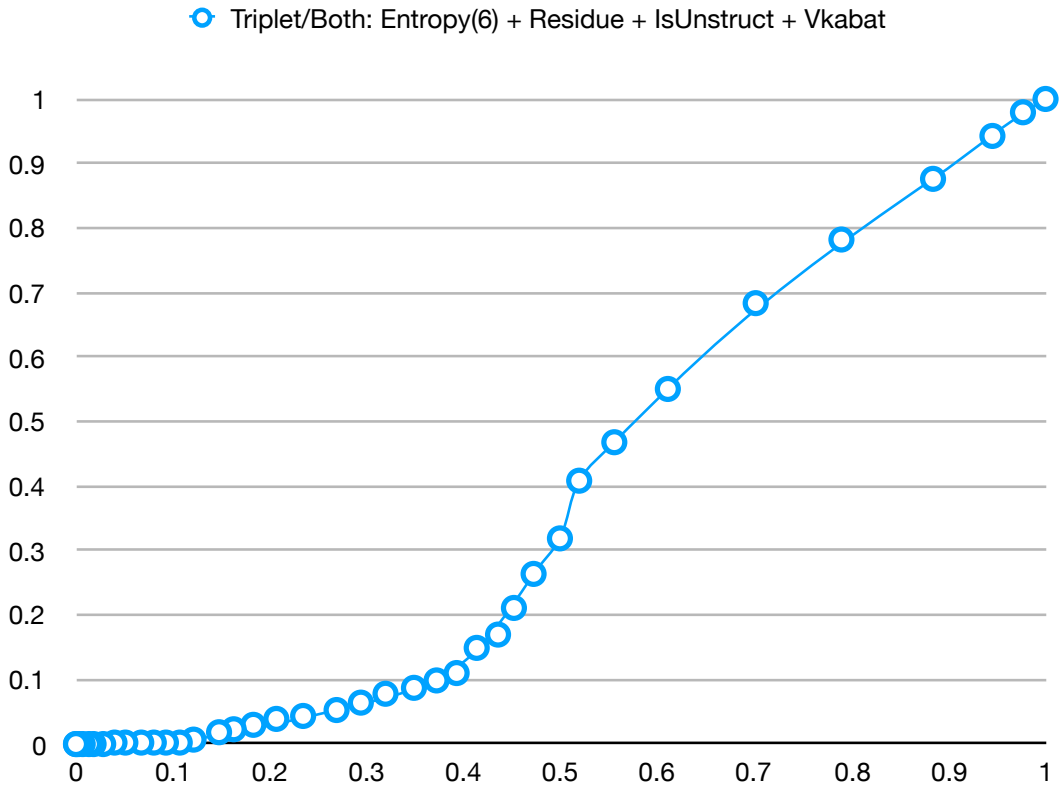
Triplet/Both: Entropy(6) + Residue + IsUnstruct + Vkabat
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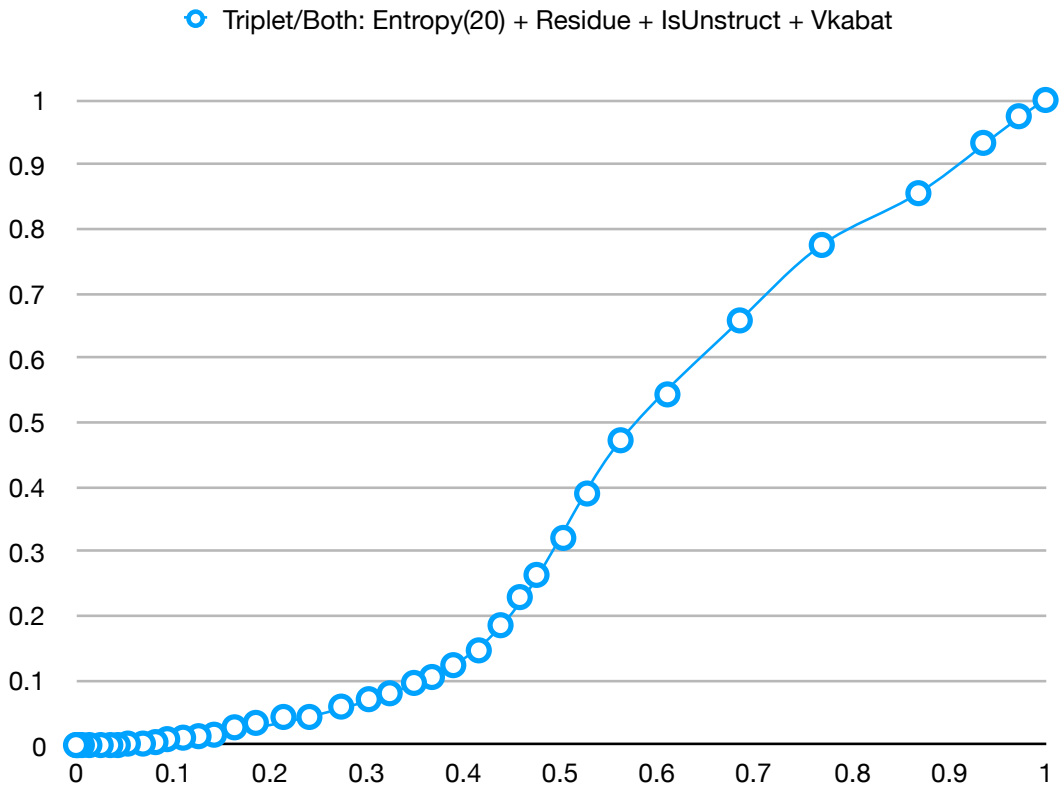
Triplet/Both: Entropy(20) + Residue + IsUnstruct + Vkabat
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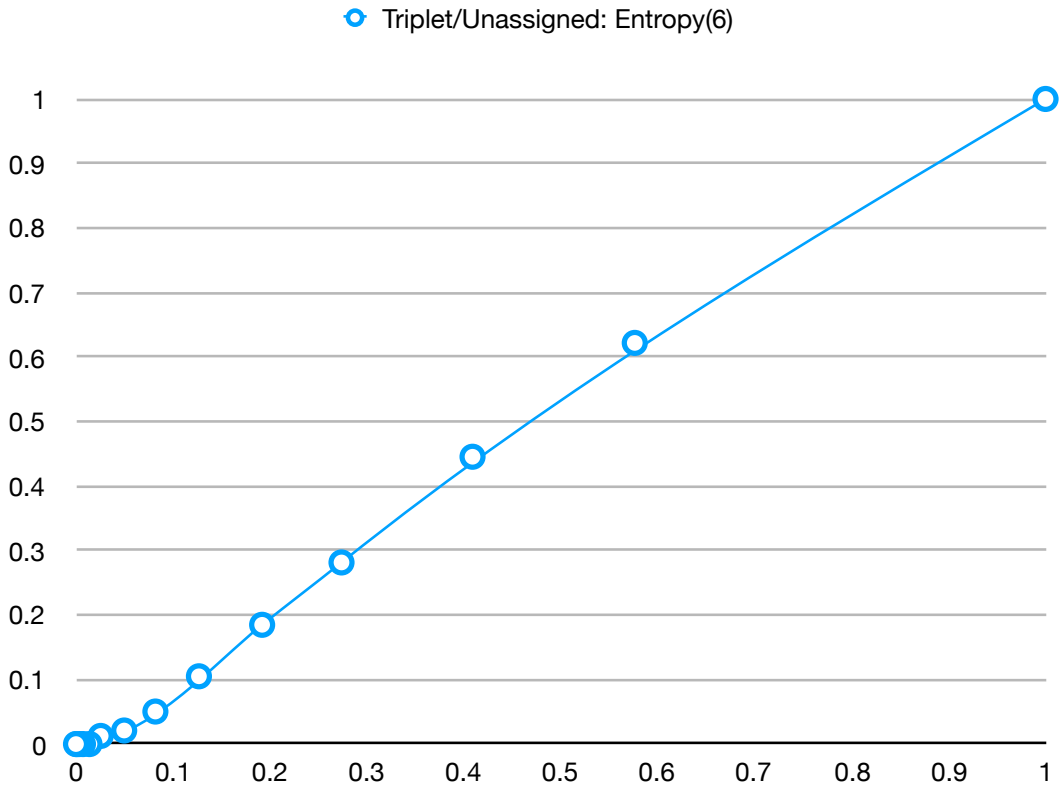
Triplet/Unassigned: Entropy(6)
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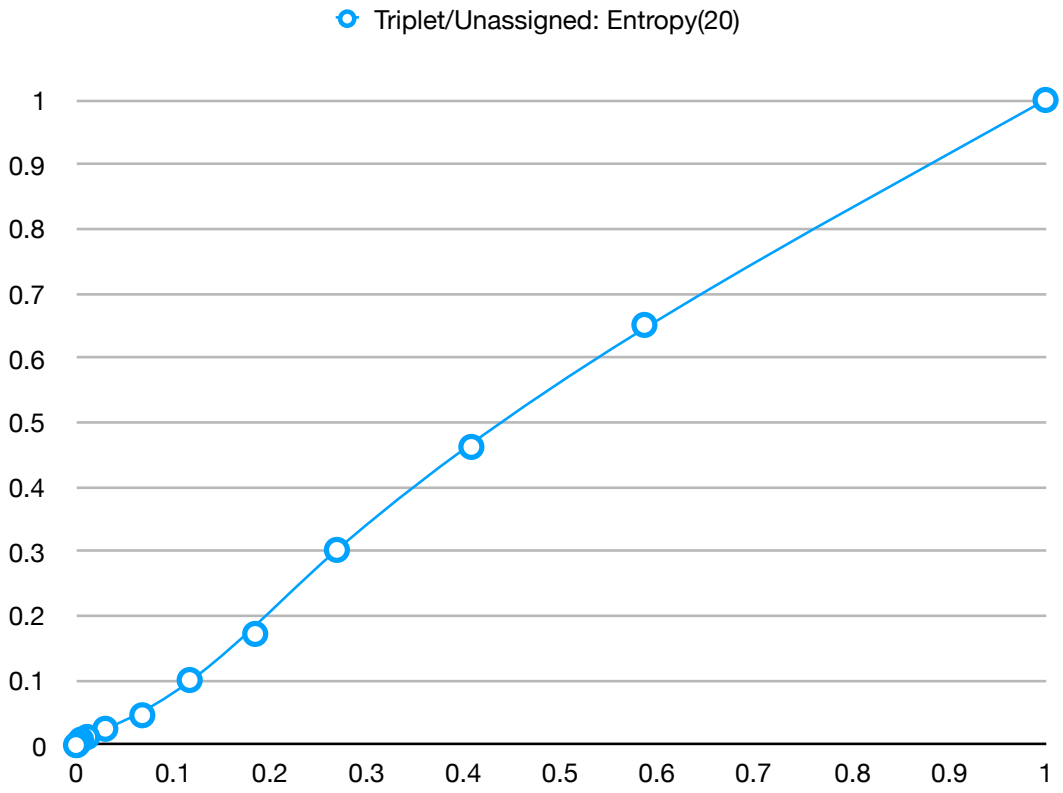
Triplet/Unassigned: Entropy(20)
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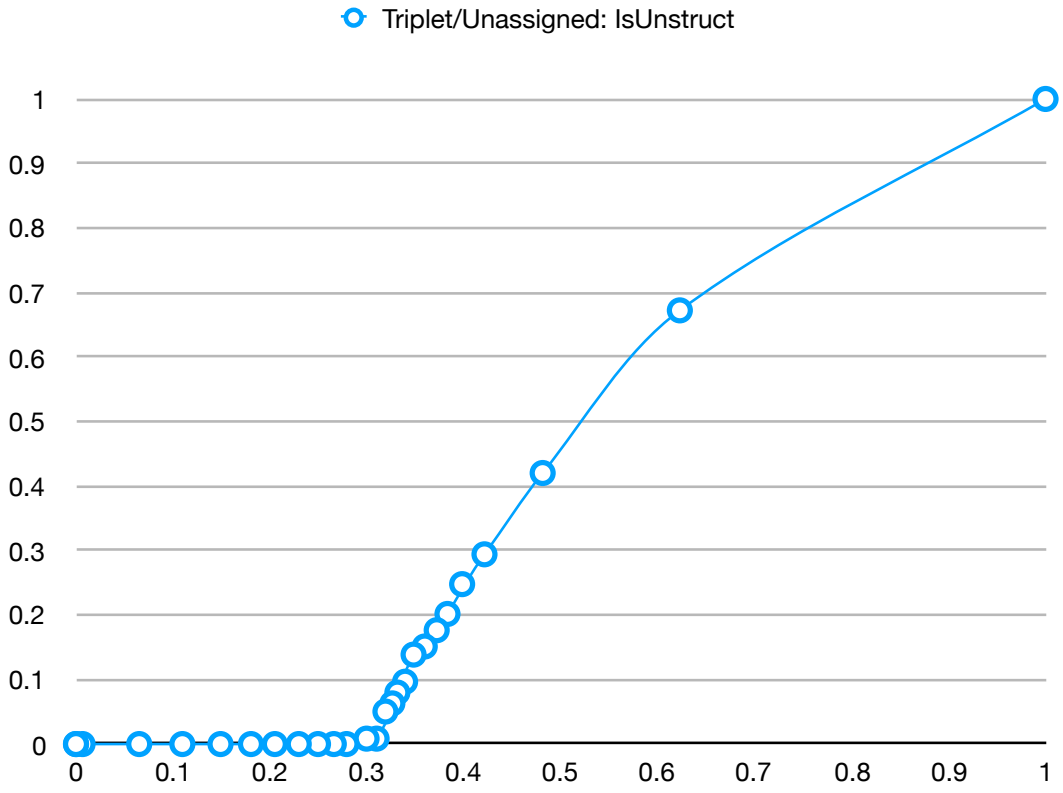
Triplet/Unassigned: IsUnstruct
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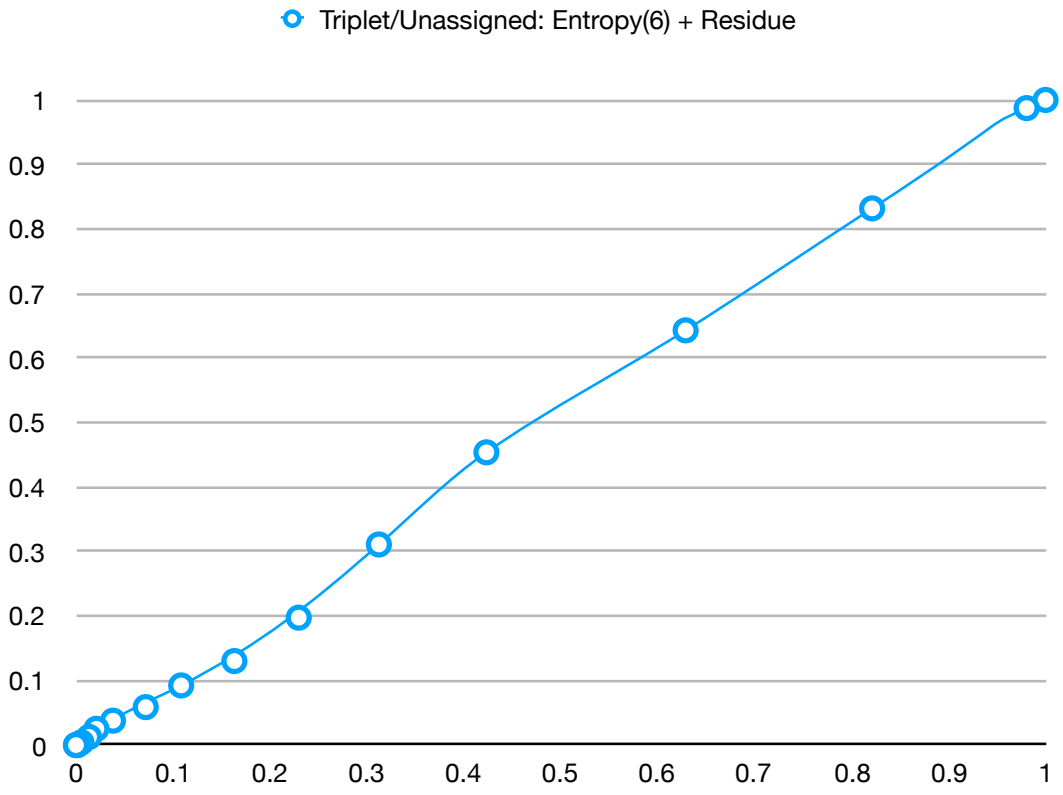
Triplet/Unassigned: Entropy(6) + Residue
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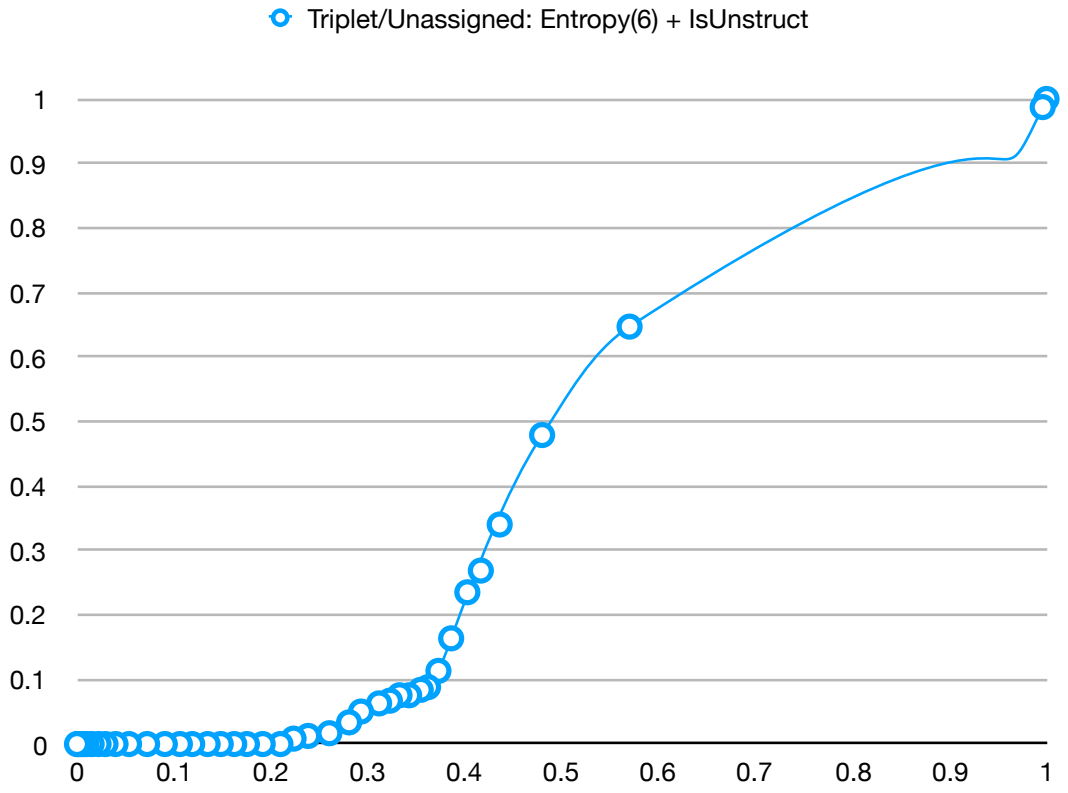
1


Triplet/Unassigned: Entropy(6) + IsUnstruct
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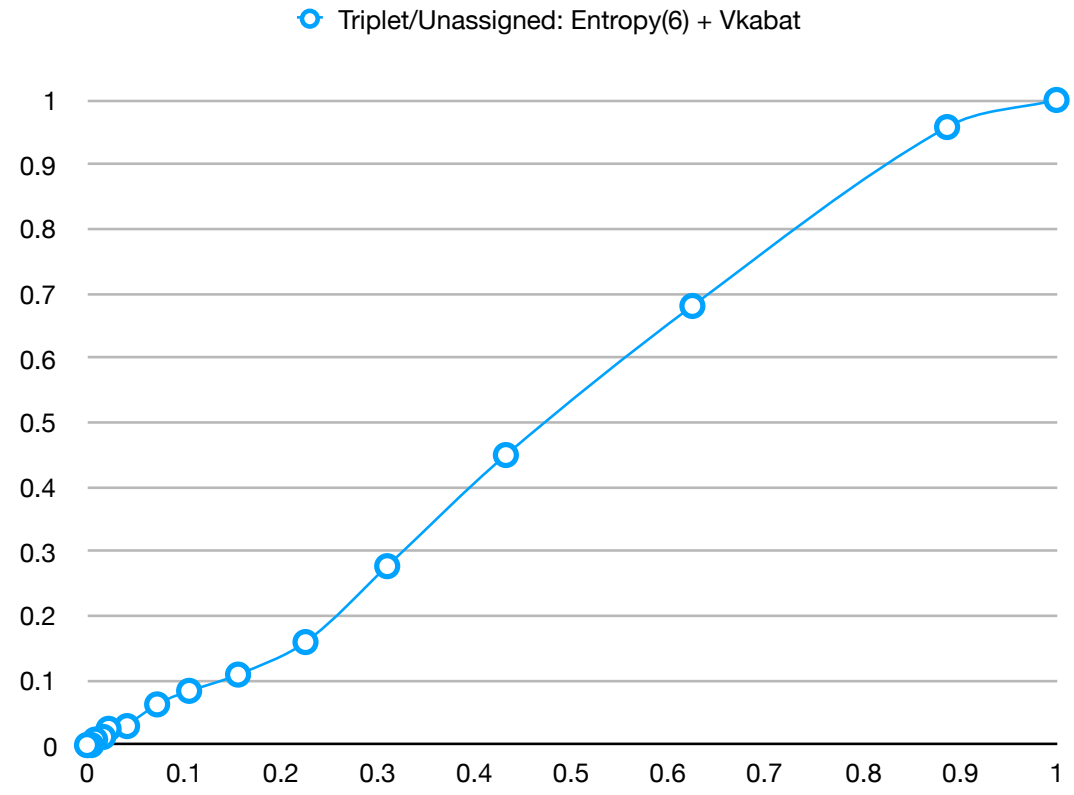
Triplet/Unassigned: Entropy(6) + Vkabat
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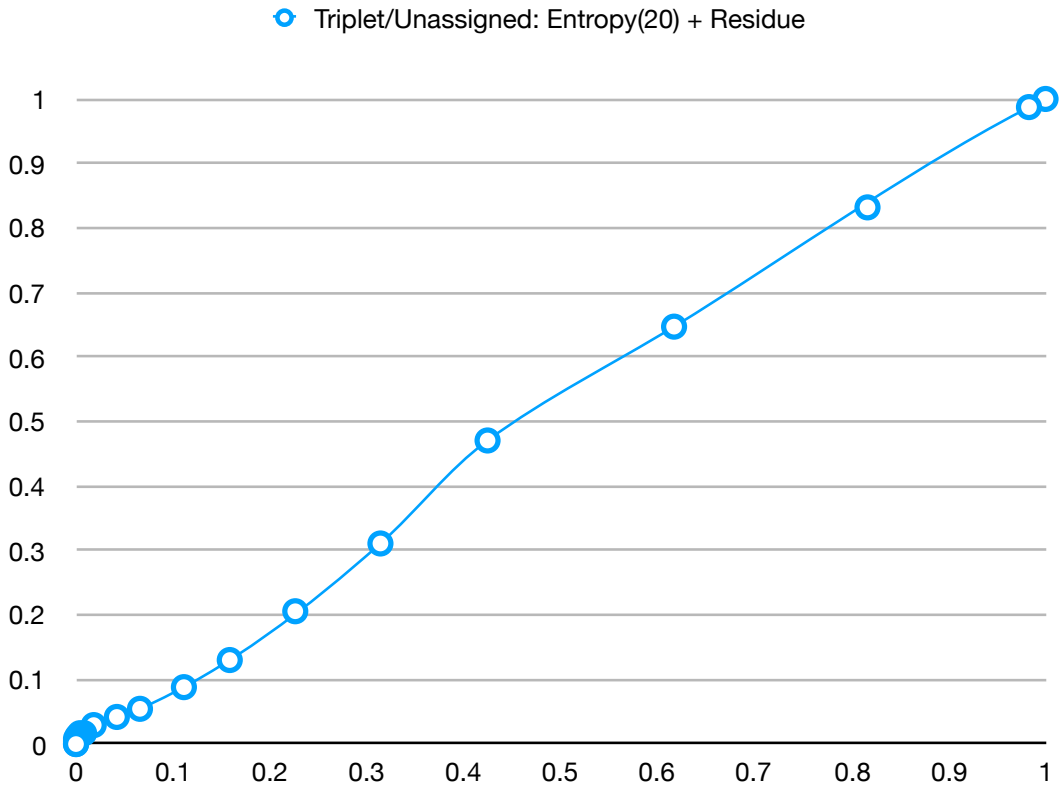
Triplet/Unassigned: Entropy(20) + Residue
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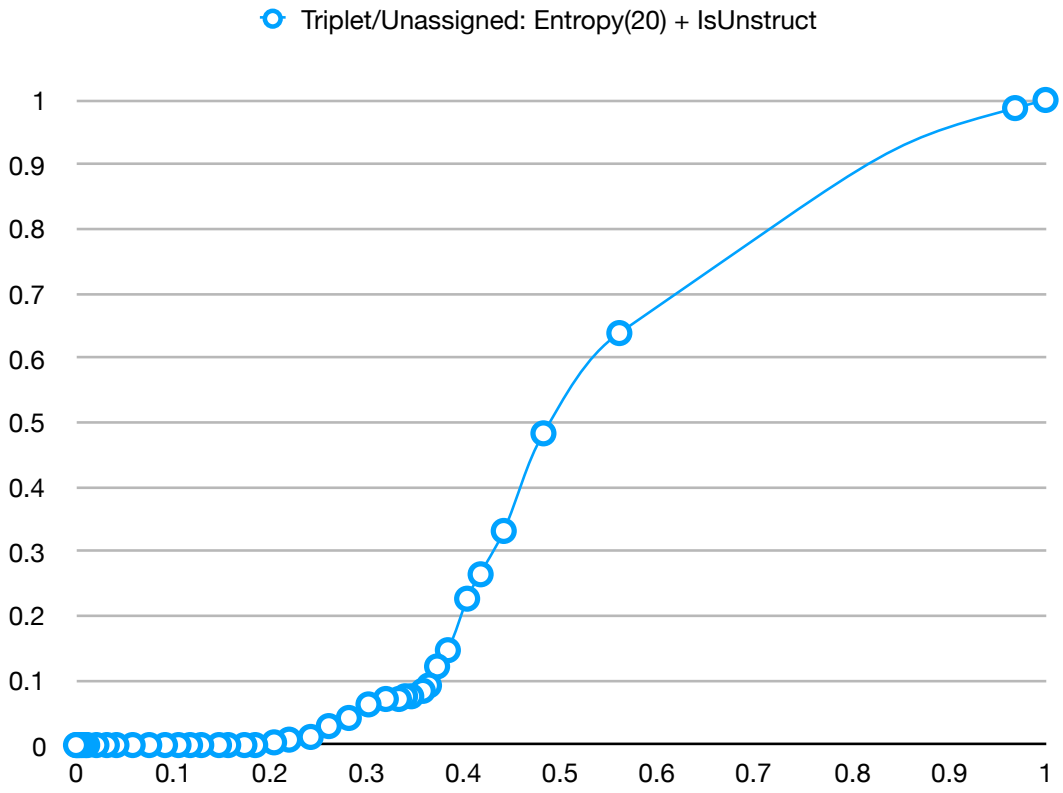
Triplet/Unassigned: Entropy(20) + IsUnstruct
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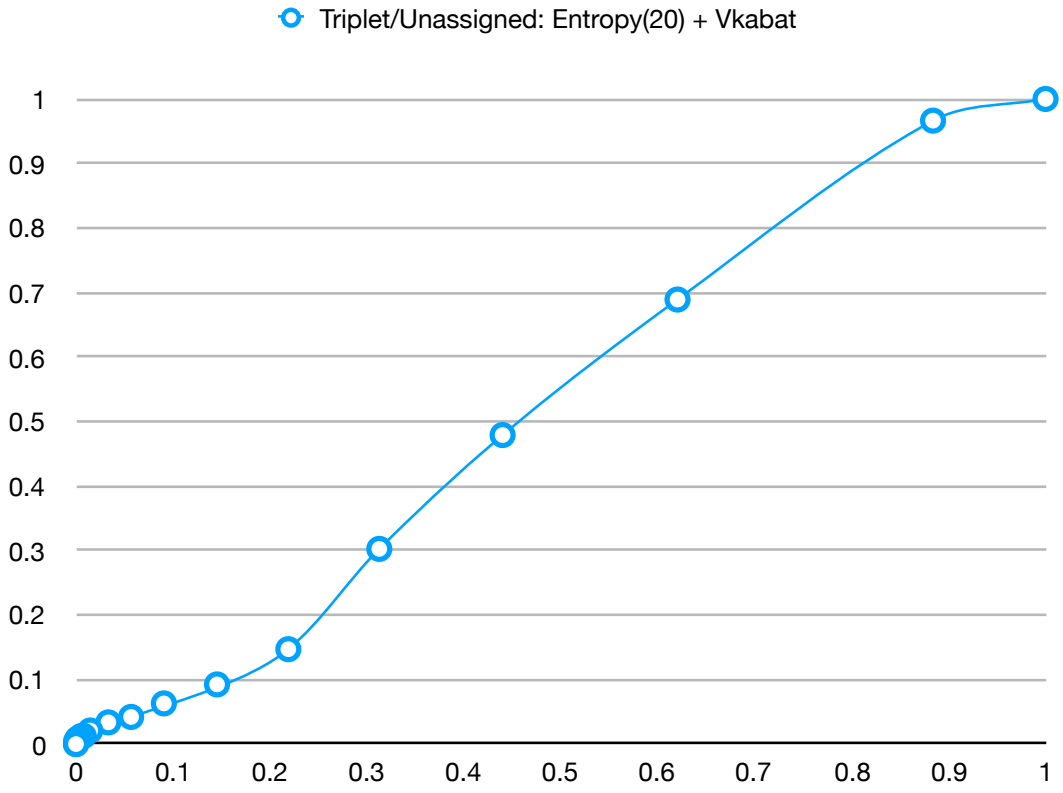
Triplet/Unassigned: Entropy(20) + Vkabat
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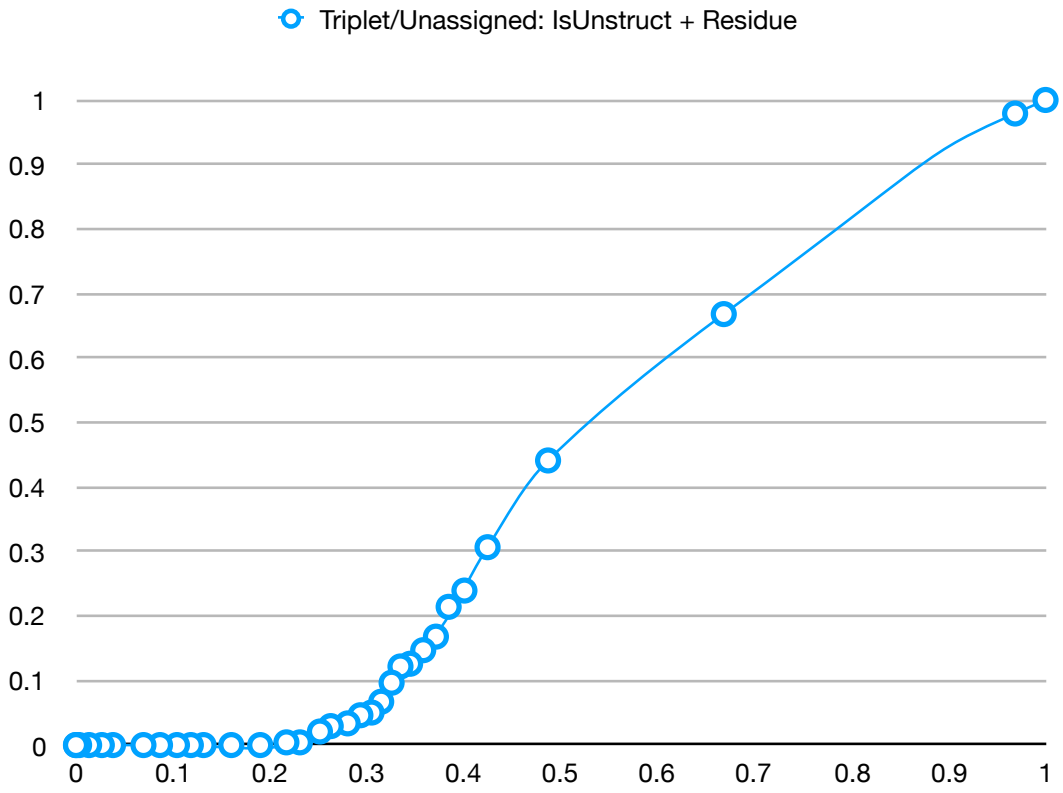
Triplet/Unassigned: IsUnstruct + Residue
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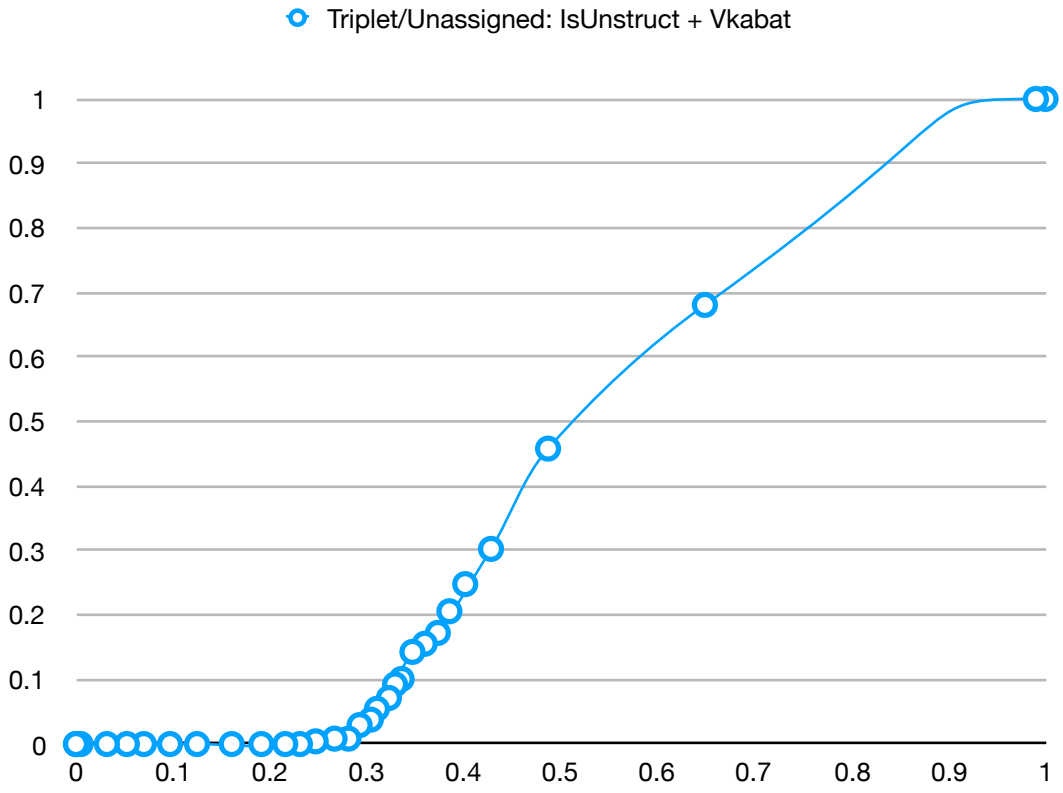
Triplet/Unassigned: IsUnstruct + Vkabat
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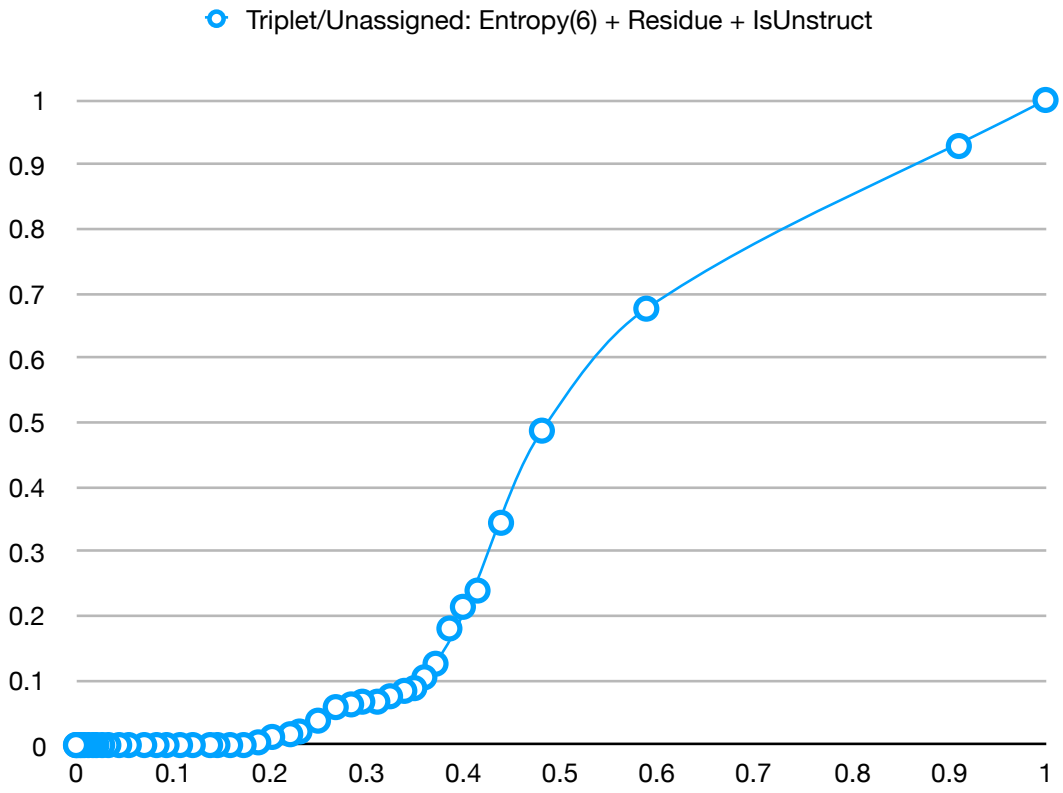
Triplet/Unassigned: Entropy(6) + Residue + IsUnstruct
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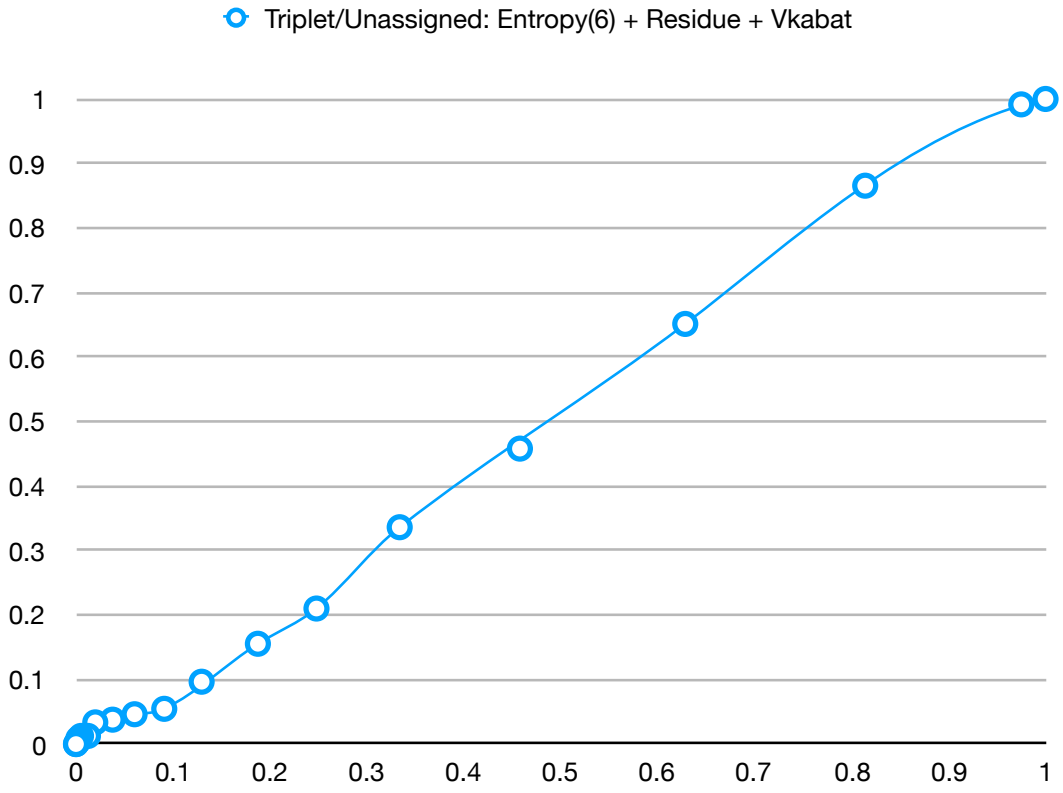
Triplet/Unassigned: Entropy(6) + Residue + Vkabat
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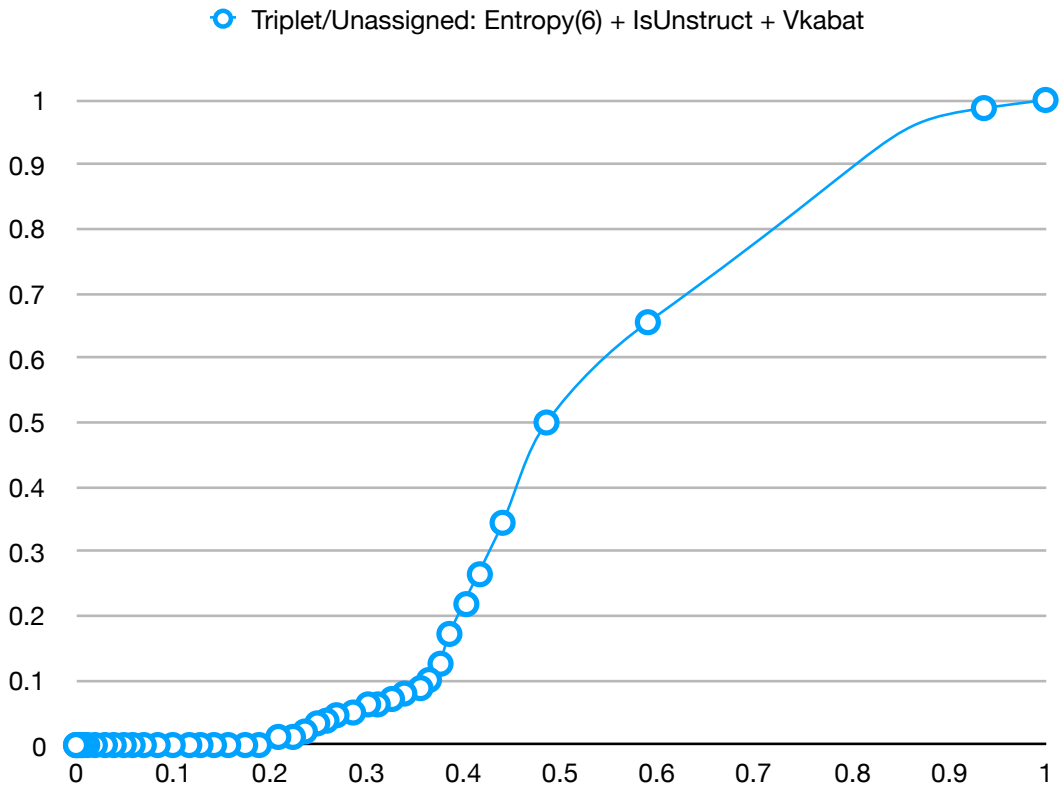
Triplet/Unassigned: Entropy(6) + IsUnstruct + Vkabat
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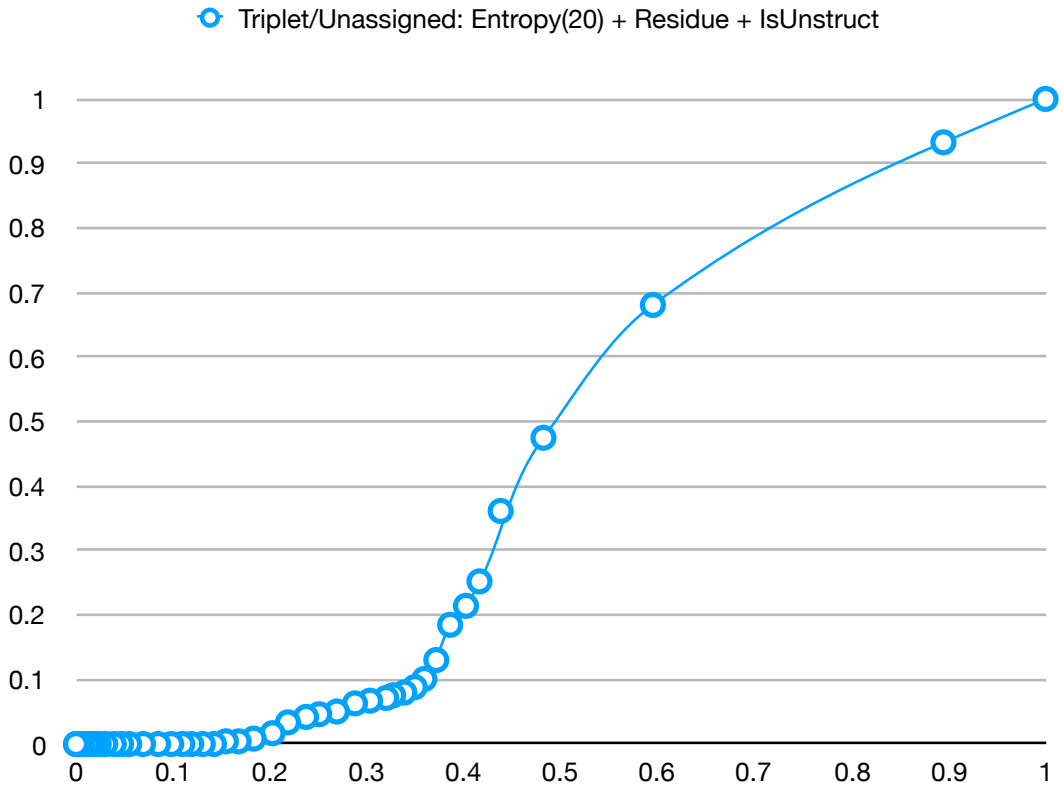
Triplet/Unassigned: Entropy(20) + Residue + IsUnstruct
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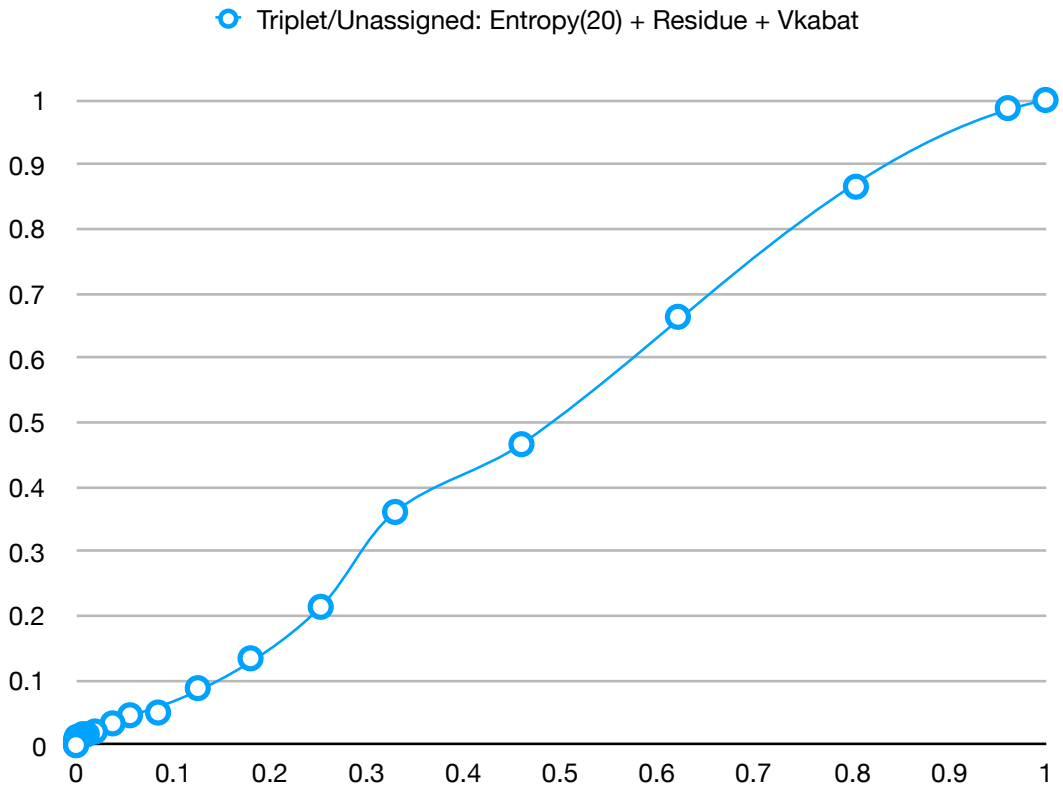
Triplet/Unassigned: Entropy(20) + Residue + Vkabat
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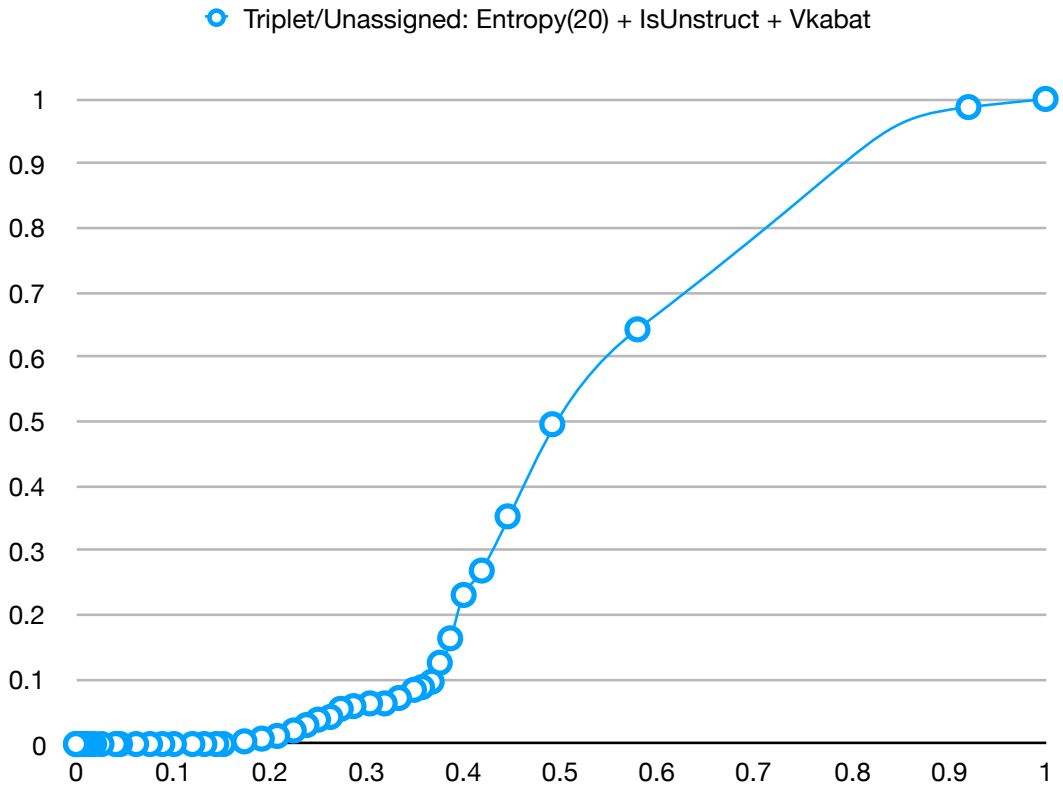
Triplet/Unassigned: Entropy(20) + IsUnstruct + Vkabat
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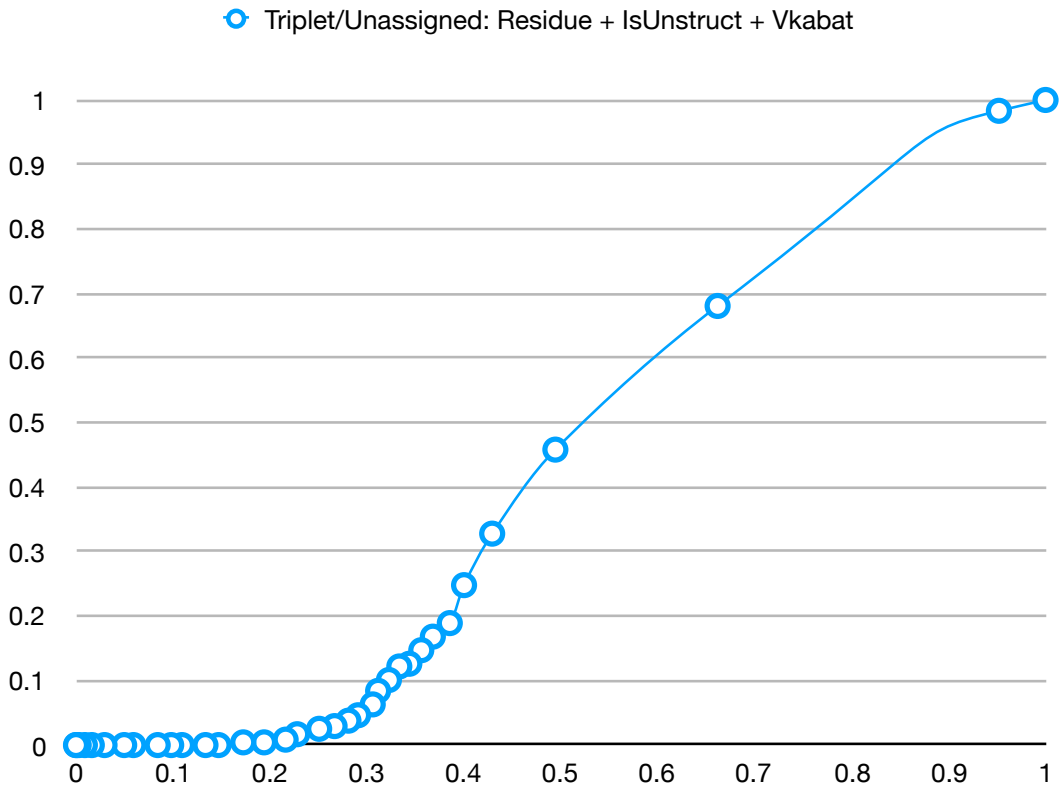
Triplet/Unassigned: Residue + IsUnstruct + Vkabat
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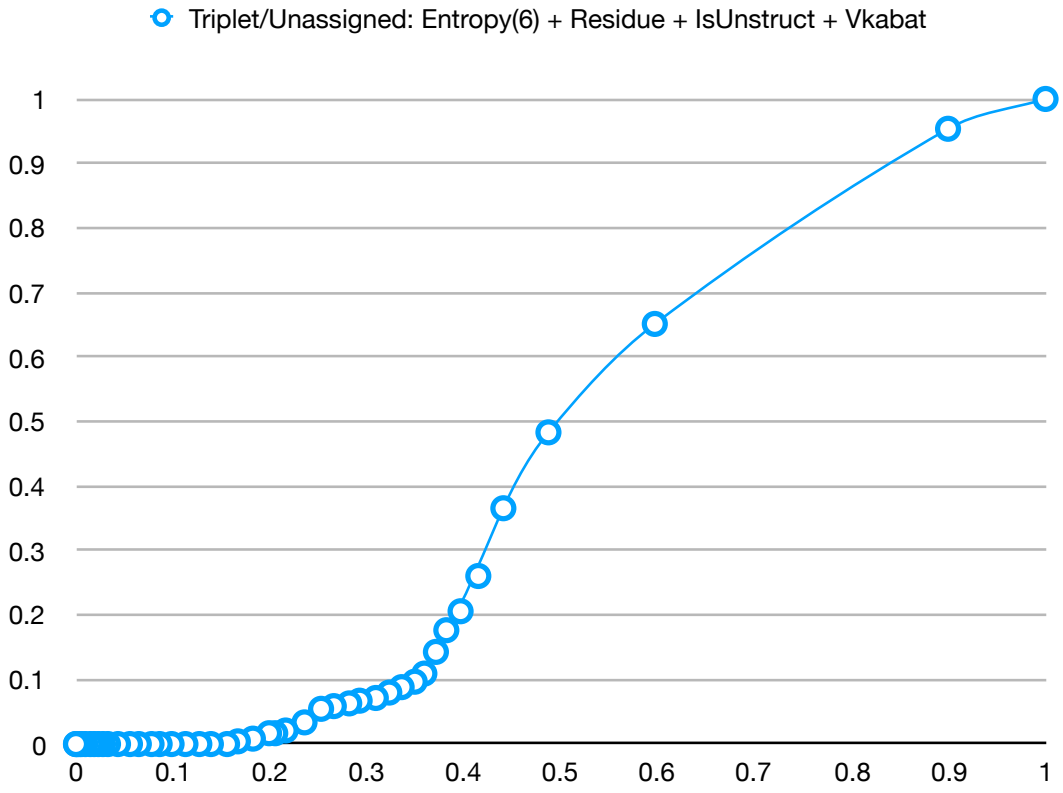
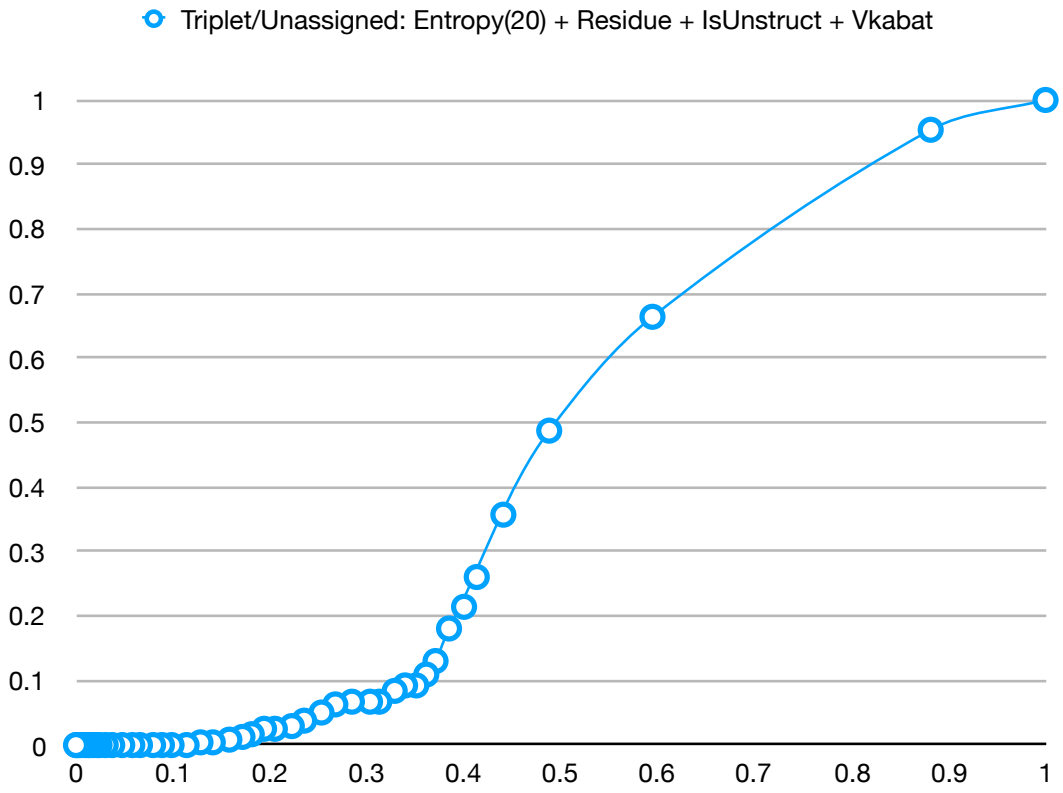
0.9
1


Triplet/Unassigned: Entropy(6) + Residue + IsUnstruct + Vkabat
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1


Triplet/Unassigned: Entropy(20) + Residue + IsUnstruct + Vkabat
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

APPENDIX D

FASTAs and Switches

In this appendix the layout is as follows:

Table D.293: Key.

Term	Definition
1st	The primary structure or residue sequence. Determined by our alignment algorithm comparing the Uniprot and DSSP sequences
2nd(r)	The raw secondary structre of the sequence, as listed in the DSSP files. '*' means that the residue was skipped in the DSSP files
2nd(s)	The secondary structre simplified to S=Sheet, H=Helix, O=Other, and D=Not Listed in DSSP.
Switch	0 = no switch 1 = assigned switch ? = unassigned switch
[#]	How many residues precede the below line of residues in the sequence, according to the DSSP file.

D.1 Learning Set

```
>1CJWA

[0]
1st   : MSTPSVHCLKPSPLHLPSGIPGSPGRQRRHTLPANEFRCLTPEDAAGVFEIEREAFISVS
2nd(r): ****************************    SSEEE   GGGHHHHHHHHIIIIIHHH
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDOOOOOOSSSOOOHHHHHHHHHHHHHHHHHH
Switch: 00000000000000000??????????????????1000000000011111111111111

[60]
1st   : GNCPLNLDEVQHFLTLCPELSLGWFVEGRLVAFIIGSLWDEERLTQESLALHRPRGHSAH
2nd(r): S  S  HHHHHHHHHH GGGEEEEEETTEEEEEEEEEE SSS  GGGGG   TT  EEE
2nd(s): OOOOOOHHHHHHHHHHOHHHSSSSSSOOSSSSSSSSSSOOOOOOHHHHHOOOOOOOSSS
Switch: ??????1111110000000010000100100000011000000001111100000000000
```

```
[120]
1st   : LHALAVHRSFRQQGKGSVLLWRYLHHVGAQPAVRRAVLMCEDALVPFYQRFGFHPAGPCA
2nd(r): EEEEEE TTSTTSSHHHHHHHHHHHHHHTSTT  EEEEEE GGGHHHHHTTTEEEEEE S
2nd(s): SSSSSSOOOOOOOOHHHHHHHHHHHHHHHOOOOOOSSSSSSOHHHHHHHHHOOOSSSSSSOO
Switch: 11000011111110000000000000011000000000000000000000000010000100

[180]
1st   : IVVGSLTFTEMHCSLRGHAALRRNSDR
2nd(r):   BTTB  EEEEEE ************
2nd(s): OOSOOSOOSSSSSSODDDDDDDDDDDD
Switch: 0110011000000000?????000000


>1GX3A

[-1]
1st   : GMAMDLGGYLTRIGLDGRPRPDLGTLHAIVAAHNRSIPFENLDPLLGIPVADLSAEALFA
2nd(r):      HHHHHHHTT  S   SSHHHHHHHHHHHHHHS EE HHHHTT      SHHHHHH
2nd(s): OOOOOHHHHHHHOOOOOOOOOOHHHHHHHHHHHHHHHOOSSOHHHHOOOOOOOOOHHHHHH
Switch: 0????11100001000000000000000000000000000000000000000000000000

[59]
1st   : KLVDRRRGGYCYEHNGLLGYVLEELGFEVERLSGRVVWMRADDAPLPAQTHNVLSVAVPG
2nd(r): HHTTT   B HHHHHHHHHHHHHHHT EEEEEEEEE TT  TT     EEEEEEEEE TT
2nd(s): HHOOOOOOSOHHHHHHHHHHHHHHHOOSSSSSSSSSOOOOOOOOOOOOSSSSSSSSSOOO
Switch: 0011000000000000000000011000000000000000000000000000000000000

[119]
1st   : ADGRYLVDVGFGGQTLTSPIRLEAGPVQQTRHEPYRLTRHGDDHTLAAQVRGEWQPLYTF
2nd(r): SSS EEE S S TT  SS EE  SSSEE  SSS EEEEEETTEEEEEEETTEEEEEEE
2nd(s): OOOOSSSOOOOOOOOOOOOSSOOOOOSSOOOOOOSSSSSSOOSSSSSSSSOOSSSSSSS
Switch: 0001000000000000000000010010100001000000000000000000000000000

[179]
1st   : TTEPRPRIDLEVGSWYVSTHPGSHFVTGLTVAVVTDDARYNLRGRNLAVHRSGATEHIRF
2nd(r):       HHHHHHHHHHHHH TT HHHHS EEEEE SSEEEEEETTEEEEEETTEEEEEE
2nd(s): OOOOOOHHHHHHHHHHHHHHOOOOHHHHOOSSSSSSOOOSSSSSSOOSSSSSSOOSSSSSS
Switch: 0000000000000000000000000000000000000100000000000001001000001
```

```
[239]
1st   : DSAAQVLDAIVNRFGIDLGDLAGRDVQARVAEVLDT
2nd(r): SSHHHHHHIIIIIS   GGGGTTS HHHHHHH TT
2nd(s): OOHHHHHHHHHHHOOOOHHHHOOOOHHHHHHHOOOO
Switch: 00100000000010000111100000000000000?

>1IB1A

[-8]
1st   : MDKNELVQKAKLAEQAERYDDMAACMKSVTEQGAELSNEERNLLSVAYKNVVGARRSSWR
2nd(r): * HHHHHHHHHHHHHTT HHHHHHHHHHHHTT     HHHHHHHHHHHHHHHHHHHHHHH
2nd(s): DOHHHHHHHHHHHHHOOOHHHHHHHHHHHHHOOOOOOOHHHHHHHHHHHHHHHHHHHHHH
Switch: ?1110000000000110000000000000110?000111?100000000000000001?

[60]
1st   : VVSSIEQKTEGAEKKQQMAREYREKIETELRDICNDVLSLLEKFLIPNASQAESKVFYLK
2nd(r): HHHHHHHH  SSSTTHHHHHHHHHHHHHHHHHHHHHHHHIIIIITTT  SHHHHHHHHH
2nd(s): HHHHHHHHOOOOOOOHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHOOOOOOHHHHHHHHH
Switch: 10000111????1111110000000000000000000000001110??11111?100

[122]
1st   : MKGDYYRYLAEVAAGDDKKGIVDQSQQAYQEAFEISKKEMQPTHPIRLGLALNFSVFYYE
2nd(r): HHHHHHHHHHH  TTHHHHHHHHHHHHHHHHHHHHHS TT HHHHHHHHHHIIII
2nd(s): HHHHHHHHHHHHOOOOHHHHHHHHHHHHHHHHHHHHHHOOOOOHHHHHHHHHHHHHH
Switch: 000000000110?1111111000000?100011111????1110000000001111?

[182]
1st   : ILNSPEKACSLAKTAFDEAIAELDTLSEESYKDSTLIMQLLRDNLTLWTSDTQGDEAEAG
2nd(r): IS  HHHHHHHHHHHHHHHHHHHTT TT   S HHHHHHHHHHHH **********
2nd(s): HOOOHHHHHHHHHHHHHHHHHHHHOOOOOOOOOOHHHHHHHHHHHHHODDDDDDDDDDD
Switch: 11?????11100000011111111??1111111?10000000111111???000?????

[242]
1st   : EGGEN
2nd(r): *****
2nd(s): DDDDD
Switch: ????0
```

```
>1N71A

[0]
1st   : MIISEFDRNNPVLKDQLSDLLRLTWPEEYGDSSAEEVEEMMNPERIAVAAVDQDELVGFI
2nd(r):  EEEE  TT HHHHHHHHHHHHHH TTTSSSTHHHHHHHHT TTSEEEEEEETTEEEEEE
2nd(s): OSSSSOOOOOHHHHHHHHHHHHHHOOOOOOOOHHHHHHHHOOOOOSSSSSSSOOSSSSSS
Switch: 0100000000000000000000110111100000000001000000000000000000000

[60]
1st   : GAIPQYGITGWELHPLVVESSRRKNQIGTRLVNYLEKEVASRGGITIYLGTDDLDHGTTL
2nd(r): EEEEEETTTEEEEEEEEE TTS SSSHHHHHHHHHHHHHHTT  EEEEEEE SSS BTT
2nd(s): SSSSSSOOOSSSSSSSSOOOOOOOOHHHHHHHHHHHHHHHHOOOOSSSSSSSOOOOOSOO
Switch: 00000000000000000001110111000000000000000000000000010000????

[120]
1st   : SQTDLYVHTFDKVASIQNLREHPYEFYEKLGYKIVGVLPNANGWDKPDIWMAKTIIPRPD
2nd(r): SSS TTSSHHHHHHT  BSS  THHHHHHTT EEEEEETTTTSTT  EEEEEEE S
2nd(s): OOOOOOOOHHHHHHOOOSOOOOOHHHHHHOOOSSSSSSOOOOOOOOOSSSSSSSOOOOOO
Switch: ??????????????????????00100000100000000000000000000000000000?

[180]
1st   : SQ
2nd(r): **
2nd(s): DD
Switch: ?0

>1S7FA

[-8]
1st   : GLVPRGSHMVEIIPVSTTLELRAADESHVPALHQLVLKNKAWLQQSLDWPQYVTSQEETR
2nd(r):   EEETTEEE EEE SSSEEEEE  GGGHHHHHHHHHHHHHHHTTSSS  ***  HHHHH
2nd(s): OOSSSOOSSSOSSSOOOOSSSSSOOHHHHHHHHHHHHHHHHHHHOOOOOOODDDOOHHHHH
Switch: 00000000110000110000000000000000000001????1????11????????10

[52]
1st   : KHVQGNILLHQRGYAKMYLIFCQNEMAGVLSFNAIEPINKAAYIGYWLDESFQGQGIMSQ
2nd(r): HHHHHHHHHHHHTS EEEEEEETTEEEEEEEEEEETTTTEEEEEEEE GGGTTSSHHHH
2nd(s): HHHHHHHHHHHHOOOSSSSSSSOOSSSSSSSSSSSOOOOSSSSSSSSOHHHOOOOHHHH
Switch: 00000000000100000000000000000000000111000000000000000000000
```

```
[112]
1st   : SLQALMTHYARRGDIRRFVIKCRVDNQASNAVARRNHFTLEGCMKQAEYLNGDYHDVNMY
2nd(r): HHHHHHHHHHHTTS  EEEEEEETT HHHHHHHHHTT EEEEEEEEEEETTEEEEEEEE
2nd(s): HHHHHHHHHHHOOOOOSSSSSSSOOOHHHHHHHHHOOOSSSSSSSSSSSSOOSSSSSSS
Switch: 00000000000100000000000000000000000000000000000010010000000

[172]
1st   : ARIIDAD
2nd(r): EEE ***
2nd(s): SSSODDD
Switch: 0000???


>1TIQA

[0]
1st   : MSVKMKKCSREDLQTLQQLSIETFNDTFKEQNSPENMKAYLESAFNTEQLEKELSNMSSQ
2nd(r): * EEEEE  GGGHHHHHHHHHHHHHHHHSTTS HHHHHHHHHHHSSHHHHHHHHH TTEE
2nd(s): DOSSSSSOOHHHHHHHHHHHHHHHHHHHHOOOOOHHHHHHHHHHHHOOHHHHHHHHHOOOSS
Switch: 00000000000000000000000001????????10000000110000000000000000

[60]
1st   : FFFIYFDHEIAGYVKVNIDDAQSEEMGAESLEIERIYIKNSFQKHGLGKHLLNKAIEIAL
2nd(r): EEEEEETTEEEEEEEEEEGGGSSS   TTEEEEEEEEE GGG SSSHHHHHHHHHHHHHH
2nd(s): SSSSSSOOSSSSSSSSSSHHHOOOOOOOOSSSSSSSSSOHHHOOOOHHHHHHHHHHHHHH
Switch: 00000000000000000000000000000000000000000000000000000000000

[120]
1st   : ERNKKNIWLGVWEKNENAIAFYKKMGFVQTGAHSFYMGDEEQTDLIMAKTLILE
2nd(r): HTT SEEEEEEETT HHHHHHHHHTT EEEEEEEEEETTEEEEEEEEEE
2nd(s): HOOOOSSSSSSSOOOHHHHHHHHHOOOSSSSSSSSSSOOSSSSSSSSSSOOOO
Switch: 00000000000000000000000000000000000000000000000000000


>1XEBA

[0]
1st   : MSLDWTCKHHADLTLKELYALLQLRTEVFVVEQKCPYQEVDGLDLVGDTHHLMAWRDGQL
2nd(r): *  EEEEEEGGG  HHHHHHHHHHHIIIIIIITT    S  S TTSTT EEEEEEETTEE
2nd(s): DOOSSSSSSHHHOOHHHHHHHHHHHHHHHHHHOOOOOOOOOOOOOOOOOSSSSSSSOOSS
Switch: 0?00000001110000000000000000000000000000000000000000010010
```

```
[60]
1st   : LAYLRLLDPVRHEGQVVIGRVVSSSAARGQGLGHQLMERALQAAERLWLDTPVYLSAQAH
2nd(r): EEEEEEE STTTTT EEEEEEEE GGGTTSSHHHHHHHHHHHHHHHHTT  EEEEEEST
2nd(s): SSSSSSSOOOOOOOOSSSSSSSSOHHHOOOOHHHHHHHHHHHHHHHHHOOOOSSSSSSOO
Switch: 00000000111100000000000001110?11100000000000000001000000000011

[120]
1st   : LQAYYGRYGFVAVTEVYLEDDIPHIGMRRA
2nd(r): THHHHHTTTEEE S  EEETTEEEEEEEE
2nd(s): OHHHHHOOOSSSOOOOSSSOOSSSSSSSSO
Switch: 111110110100111101??11000001?


>2B5GA

[0]
1st   : MAKFVIRPATAADCSDILRLIKELAKYEYMEEQVILTEKDLLEDGFGEHPFYHCLVAEVP
2nd(r): *   EEEE  GGGHHHHHHHHHHHHT ****      HHHHHHHHSSSS S EEEEEE
2nd(s): DOOOSSSSOOHHHHHHHHHHHHHHHHOODDDDOOOOOOOHHHHHHHHOOOOOOOSSSSSSOO
Switch: 0??00000000000000000000111????110000110000001????0000000000

[60]
1st   : KEHWTPEGHSIVGFAMYYFTYDPWIGKLLYLEDFFVMSDYRGFGIGSEILKNLSQVAMRC
2nd(r): GGG  TT   EEEEEEEEEEEETTTEEEEEEEEEEE GGG SSSHHHHHHHHHHHHHHHH
2nd(s): HHHOOOOOOOSSSSSSSSSSSOOOSSSSSSSSSSSOHHHOOOOHHHHHHHHHHHHHHHH
Switch: 111??000000000000000000000000000000000000000000000000000001

[120]
1st   : RCSSMHFLVAEWNEPSINFYKRRGASDLSSEEGWRLFKIDKEYLLKMATEE
2nd(r): T SEEEEEEETT HHHHHHHHTTT EEHHHHHTEEEEEEEHHHHHHHH **
2nd(s): OOOSSSSSSSOOOHHHHHHHHOOOOSSHHHHHOSSSSSSSHHHHHHHHODD
Switch: 000100111100000000011000111111?1111111000000111??


>2BL1A

[0]
1st   : MSASIRDAGVADLPGILAIYNDAVGNTTAIWNETPVDLANRQAWFDTRARQGYPILVASD
2nd(r): ** EEEE  GGGHHHHHHHHHHHHH SSS   S   HHHHHHHHHHHHHT  EEEEE
2nd(s): DDOSSSSOOHHHHHHHHHHHHHHHHHHOOOOOOOOOOOHHHHHHHHHHHHHHOOOSSSSSO
Switch: 0??10000000000000000000000000000000000000000000000000000000000
```

```
[60]
1st   : AAGEVLGYASYGDWRPFEGFRGTVEHSVYVRDDQRGKGLGVQLLQALIERARAQGLHVMV
2nd(r): TT    EEEEEEESSSSGGGTTEEEEEEEE TTSTTSSHHHHHHHHHHHHHHTT  EEE
2nd(s): OOOOOOSSSSSSSOOOOHHHOOSSSSSSSSOOOOOOOOHHHHHHHHHHHHHHHOOOOSSS
Switch: 00001100000000000000000000000001110000000000000000000000000

[120]
1st   : AAIESGNAASIGLHRRLGFEISGQMPQVGQKFGRWLDLTFMQLNLDPTRSAP
2nd(r): EEEETT HHHHHHHHHTT EEEEEEEEEEEETTEEEEEEEEEES TT
2nd(s): SSSSOOOHHHHHHHHHOOOSSSSSSSSSSSSOOSSSSSSSSSSOOOOOOOO
Switch: 00000000000000010000000000000000000000000000000000


>2FIAA

[0]
1st   : MKIRVADEKELPMILQFLTEVKAYMDVVGITQWTKDYPSQGDIQEDITKKRLYLLVHEEM
2nd(r):   EEE  GGGTTHHHHHHHHHHHHHHHT     SSSS HHHHHHHHHTT EEEEEETTE
2nd(s): OOSSSOOHHHOOHHHHHHHHHHHHHHHHOOOOOOOOOOOHHHHHHHHHOOOSSSSSSOOS
Switch: 00000000001100000000000000000000000000000000000000011001

[60]
1st   : IFSMATFCMEQEQDFVWLKRFATSPNYIAKGYGSLLFHELEKRAVWEGRRKMYAQTNHTN
2nd(r): EEEEEEEEE TT SEEEEEEEEE GGGTTTTHHHHHHHHHHHHHHTTT  EEEEEEETT
2nd(s): SSSSSSSSSOOOOOSSSSSSSSSOHHHOOOOHHHHHHHHHHHHHHHOOOOOSSSSSSSOOO
Switch: 11000000100000000000000000010000000000000000000000000000000

[120]
1st   : HRMIRFFESKGFTKIHESLQMNRLDFGSFYLYVKELENQSIV
2nd(r): HHHHHHHHHTT EEEEEE  TT GGG  EEEEEEE  *****
2nd(s): HHHHHHHHHOOOSSSSSSOOOOOHHHOOSSSSSSSOODDDDD
Switch: 00000000010000000000000000000000000??000


>2JLMA

[0]
1st   : MFSPSTTTLFRFVECTEDQHALEILEILNDAIINSTALYDYKPRSKESMAAWFATKRQNN
2nd(r): *****    EEEEE  HHHHHHHHHHHHHHHHHH SSS  SS   HHHHHHHHHHHHHTT
2nd(s): DDDDDOOOOSSSSSOOHHHHHHHHHHHHHHHHHHHOOOOOOOOOOOHHHHHHHHHHHHHOO
Switch: ?????1111100000000000000000000000000000000000110000000000110
```

```
[60]
1st   : FPIIGAVNEVGQLLGFASWGSFRAFPAYKYTVEHSVYIHKDYRGLGLSKHLMNELIKRAV
2nd(r):   EEEEEETTS EEEEEEEEESSSSGGGTTEEEEEEEE TTSTTSSHHHHHHHHHHHHHH
2nd(s): OOSSSSSSOOOOSSSSSSSSSOOOOHHHOOSSSSSSSSOOOOOOOOHHHHHHHHHHHHHH
Switch: 00000001000000000000000000000000000000011100000000000000000

[120]
1st   : ESEVHVMVGCIDATNVASIQLHQKLGFIHSGTIQQAGFKFGRWLDAAFYQLTLDTPLHPQ
2nd(r): HTT  EEEEEEETT HHHHHHHHHTT EEEEEEEEEEEETTEEEEEEEEEEE S  SS
2nd(s): HOOOOSSSSSSSOOOHHHHHHHHHOOOSSSSSSSSSSSSOOSSSSSSSSSSOOOOOOOO
Switch: 00000000000000000000000000000000000000000000000000000000000

[180]
1st   : DD
2nd(r):
2nd(s): OO
Switch: 0?


>2Q4VA

[0]
1st   : MASVRIREAKEGDCGDILRLIRELAEFEKLSDQVKISEEALRADGFGDNPFYHCLVAEIL
2nd(r): ** EE  B  GGGHHHHHHHHHHHHHHHT ****   HHHHHHHHTSSS S EEEEEEE
2nd(s): DDOSSOOSOOHHHHHHHHHHHHHHHHHHHOODDDDOOOHHHHHHHHOOOOOOOSSSSSSSO
Switch: 0?0101100000000000000000000100????000000000001000000000000001?

[60]
1st   : PAPGKLLGPCVVGYGIYYFIYSTWKGRTIYLEDIYVMPEYRGQGIGSKIIKKVAEVALDK
2nd(r): *******  EEEEEEEEEEEETTTEEEEEEEEEEE GGGTTSSHHHHHHHHHHHHHHHT
2nd(s): DDDDDDDOOSSSSSSSSSSSSSOOOSSSSSSSSSSSOHHHOOOOHHHHHHHHHHHHHHHO
Switch: 0000000??1000000000001000100000000000000000000000000000000001

[120]
1st   : GCSQFRLAVLDWNQRAMDLYKALGAQDLTEAEGWHFFCFQGEATRKLAGK
2nd(r): T  EEEEEE SS HHHHHHHHHTT EEHHHHT EEEEEEETHHHHHHT *
2nd(s): OOOSSSSSSOOOOHHHHHHHHHOOOSSHHHHOOSSSSSSSOHHHHHHOOD
Switch: 00000000010001100000011000011111010000011000000107
```

```
>2REEA

[0]
1st   : MLELINRYEHGFVYIPVILACREKGLFELIKKKRITHRQIANTLGANTGNLQVALTMMES
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 00000000000000000000000000000000000000000000000000000000000

[60]
1st   : LGWLSKNEADEYSLKDNCQAYLSIPEEILYLYNLPIESYLLGKEKPGIIKNWIELSQQQW
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 00000000000000000000000000000000000000000000000000000000000

[120]
1st   : NINDRTIADLLDGVLIIPIMLGLHKHNLLAVDEDKPLFYNVTPHIREELSRLFIAKGWAD
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 00000000000000000000000000000000000000000000000000000000000

[180]
1st   : KSLIKVQKHSQKSNKNKNYLCLTDIGKCLGQRTIIKSISLNCFENNYYNLRHPKIEDLRD
2nd(r): ******************************************  EEEE   GGGHHH
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDOOSSSSOOOHHHHHH
Switch: 00000000000000000000000000000000000000000???0000000000000000

[240]
1st   : LIALETLCWSENLQVDNEEIYRRIFKIPQGQFILELEDKIVGAIYSQRIDNPQLLDNKTC
2nd(r): HHHHHHHHS TTT   HHHHHHHHHH GGG EEEEESS EEEEEEEEEES GGGGTT  T
2nd(s): HHHHHHHHOOOOOOOOHHHHHHHHHHHOHHHOSSSSSOOOSSSSSSSSSOOHHHHOOOOO
Switch: 00000000001110000000000000000100000001000000000000000000000

[300]
1st   : TQVPLLHTESGVVVQLLAVNILPELQNQGLGDRLLEFMLQYCAQISGVEKVVAVTLCRNY
2nd(r): TTGGGG  TT SEEEEEEEEE GGG SSSHHHHHHHHHHHHHTTSTT  EEEEEE  SSG
2nd(s): OOHHHHOOOOOOSSSSSSSSSOHHHOOOOHHHHHHHHHHHHHOOOOOOOSSSSSSOOOOH
Switch: 00100000000000000000011100000000000000000100000000000000000
```

```
[360]
1st   : PDYSPMPMAEYIHQKNESGLLVDPLLRFHQIHGAKIEKLLPGYRPKDWENQTCGVLVSYD
2nd(r): GGTTTS HHHHTT B TTS BSSHHHHHHHHTT EEEEEETTS TT GGGTT EEEEEE
2nd(s): HHOOOOOHHHHOOOSOOOOOSOOHHHHHHHHHOOOSSSSSSOOOOOOOHHHOOOSSSSSSO
Switch: 00100000000000000000000000000100100000000000001110000000000

[420]
1st   : IQHRQRFDGATVEKNRQTKVKLTEDIDEVVASCVRKVMHQKKSFDAQRALMEMGIESLEL
2nd(r):  TT ************************************************************
2nd(s): OOOODDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 000000000000000000000000000000000000000000000000000000000000

[480]
1st   : LELRYLLQKKLGVEIDPNLFFKYGTAAAIASYFKGETTERSGEVSEVLPKPEAIKTDSGF
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 000000000000000000000000000000000000000000000000000000000000

[540]
1st   : STAQLENGVAIIGMACRFPGDADSPQQYWSLLHDGIDGITEVPPTRWDIEQYYHPEKNQP
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 000000000000000000000000000000000000000000000000000000000000

[600]
1st   : GKIANRYGGFLTEVDKFEPDFFRISAREALYMDPQQRLLLEEHWKALEDAGINPESLSGT
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 000000000000000000000000000000000000000000000000000000000000

[660]
1st   : ETGIFVGIAFHDYERLQDKYYQEQDLNIYFATGSSTAIGAGRLSYFFQLNGPSITVDTAC
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 000000000000000000000000000000000000000000000000000000000000

[720]
1st   : SSSLSAVHLACQSIRNGECQLALASGVNLLLSPELSISFSQAGMLSPDGRCKTFDAAANG
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 000000000000000000000000000000000000000000000000000000000000
```

```
[780]
1st   : YVRSEGCGVVVLKSLKQAIADNDRILAVVRGTAINQDGASNGLTAPNQSAQEAVLKRALS
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 000000000000000000000000000000000000000000000000000000000000

[840]
1st   : VAGVSANQISYVEAHGTGTSLGDPVEIKAIEAVYGKDRSADRPLMIGSVKTNIGHTEAAA
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 000000000000000000000000000000000000000000000000000000000000

[900]
1st   : GIAGLIKVVLSLQNQYIPPHLHWKQLNPYISLAGIPGVIPTEGKVWEQYEGDETRVAALS
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 000000000000000000000000000000000000000000000000000000000000

[960]
1st   : SFGFSGTNSHAIVEEAPEGRSQEPGARSQEPGARSQEPPYLLTVSAKKEQALKELVSSYQ
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 000000000000000000000000000000000000000000000000000000000000

[1020]
1st   : HHLETNPELELADVCYTANTGRADFNHRLAIIATNPQQLTNKLRQYQAGEEESGVFSGQL
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 000000000000000000000000000000000000000000000000000000000000

[1080]
1st   : SHSSSPAKVAFLFTGQGSQYVQMGRQLYQTQPVFRQVLDQCDELLRPYLERPLLEVLYPQ
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 000000000000000000000000000000000000000000000000000000000000

[1140]
1st   : DTPNSNSYLLDQTAYTQPTLFALEYALCKLWESWGIKPQVVMGHSVGEYVAATIAGVLSL
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 000000000000000000000000000000000000000000000000000000000000
```

```
[1200]
1st   : EDGLKLIALRGRLMQQLPAGGEMVSVMASKSQVKDAIANHTKQVTIAAINGPESVVISGE
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 00000000000000000000000000000000000000000000000000000000000

[1260]
1st   : AGAIQAIVTKLESKLIKTKQLQVSHAFHSPLMTPMLAEFAAVAQQITYHQPRIPVISNVT
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 00000000000000000000000000000000000000000000000000000000000

[1320]
1st   : GTIADKSIATADYWVEHVVKPVRFVAGIKTLAEQDIRIFLEIGPKPVLLVMGRECLIGSK
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 00000000000000000000000000000000000000000000000000000000000

[1380]
1st   : KIWLPSLRPGKPDWLQMLQSLGQLYVQGVKVDWLGFYPDDAPQKVVLPTYPWQRKRYWIS
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 00000000000000000000000000000000000000000000000000000000000

[1440]
1st   : DLQQYKNKGKNGKVAPQVASDNNQSKNSVVTNNSSGSKMLPGIKESEQPRIKEREQPRIK
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 00000000000000000000000000000000000000000000000000000000000

[1500]
1st   : ESEQDARTTINIQKSDAPDIEQPQRRLSNPASLSLSKTTVAKQQPAKRELAQLRVPLTQV
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 00000000000000000000000000000000000000000000000000000000000

[1560]
1st   : EPAQITQQYLESEKITQTLGKALHQDILINQKTTKEPKTMNREQVEQLKQEYEEKGYCQI
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 00000000000000000000000000000000000000000000000000000000000
```

```
[1620]
1st   : KKIFDFSAIKTIQKTLDQAKQESQISKEKVTLKLGGIDDIDTNDHAYDLVKYDFVSSFIQ
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 000000000000000000000000000000000000000000000000000000000000

[1680]
1st   : EKLALLNYITGKNLMIMHNALFSVEPNHKGLPWHVGVGSFSFTKTEDFGASIWIPLDKIT
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 000000000000000000000000000000000000000000000000000000000000

[1740]
1st   : KEHRGGMQYVSTKIFPGQFYYSVFDLHLKNNIKWDESQGDLNEYVANANTIYNKITEDVI
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 000000000000000000000000000000000000000000000000000000000000

[1800]
1st   : DYTIKDGYEEDEYNLGDAFFFNKYVLHQSVPLKPGLHKLRRAFVIRLVDYDTRVDEERLG
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 000000000000000000000000000000000000000000000000000000000000

[1860]
1st   : LFSKYSQLHSRYYKTLPRYNKDSVLVMVSRAVQKGLKSPYLRDIPHVQQTLAARMAAGAI
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 000000000000000000000000000000000000000000000000000000000000

[1920]
1st   : SFEETPSISSAPQTQQPLKTLQPLRTPQVNQVNLSEIKQVLKQQLAEALYTEESEIAEDQ
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 000000000000000000000000000000000000000000000000000000000000

[1980]
1st   : KFVDLGLDSIVGVEWTTTINQTYNLNLKATKLYDYPTLLELSGYIAQILSSQGTKPISSS
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 000000000000000000000000000000000000000000000000000000000000
```

```
[2040]
1st   : SQTQQSLKTLQPLPTPQVNQVNLSEIKQVLKQQLAEALYTEESEIAEDQKFVDLGLDSIV
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 000000000000000000000000000000000000000000000000000000000000

[2100]
1st   : GVEWTTTINQTYNLNLKATKLYDYPTLLELAAYIAQTLASQGTKPQVSQQPLKTLQPLPQ
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 000000000000000000000000000000000000000000000000000000000000

[2160]
1st   : PQVNLSEIKQVLKQQLAEALYTEESEIAEDQKFVDLGLDSIVGVEWTTTINQTYNLNLKA
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 000000000000000000000000000000000000000000000000000000000000

[2220]
1st   : TKLYDYPTLLELAPYIAQEIAATGGSKLFQGNGNGGHPQESLPNNGSPVNSSEEMDPKLR
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 000000000000000000000000000000000000000000000000000000000000

[2280]
1st   : LRAILNKVAKKELTIQEANKLVQQIKKQVTV
2nd(r): ********************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 000000000000000000000000000000


>2VFBA

[0]
1st   : MALDLTGYLDRINYRGATDPTLDVLRDLVSAHTGAIAFENLDPLMGVPVDDLSAEALADK
2nd(r): *** HHHHHHHTT  S  SSSHHHHHHHHHHHHHHS EE HHHHTT      SHHHHHII
2nd(s): DDDOHHHHHHHOOOOOOOOOOHHHHHHHHHHHHHHOOSSOHHHHOOOOOOOOOHHHHHHH
Switch: 00?010000000007000000000000000000000000000000000000000000000
```

```
[60]
1st   : LVDRRRGGYCYEHNGLIGYVLAELGYRVRRLAGRVVWLAPPDAPTPAQTHTVLAVTFPGC
2nd(r): IIIT   B HHHHHHHHHHHHHHHT EEEEEEEEE TT  TTS    S EEEEEEE TT
2nd(s): HHHOOOOSOHHHHHHHHHHHHHHHOOSSSSSSSSSOOOOOOOOOOOOOOSSSSSSSOOOO
Switch: 00000000000000000000000000000000000000000000000011000000000000

[120]
1st   : QGPYLVDVGFGGMTPTAPLRLETGTVQQTALEPYRLDDRGDGLVLQAMVRDEWQALYEFS
2nd(r): SS EEE S SGGG  SS EES BS  EE SSSEEEEEEETTEEEEEEEETTEEEEEEEE
2nd(s): OOOSSSOOOOHHHOOOOOSSOOSOOOSSOOOOSSSSSSSOOSSSSSSSSOOSSSSSSSSO
Switch: 00000000001110000000001001010000100000000000000100100000000

[180]
1st   : TLTRPQVDLRVGSWFVSTHPTSHFVTGLMAATVADDARWNLMGRNLAIHRRGGTEKILLE
2nd(r):  S   HHHHHHHHHHHHH TT HHHHS EEEEE SS EEEEETTEEEEEETTEEEEEE
2nd(s): OOOOOHHHHHHHHHHHHHHOOOOHHHHOOSSSSSOOOOSSSSSOOSSSSSSOOSSSSSSOO
Switch: 00000000000000000000000000000000100100000000000010011000000

[240]
1st   : DAAAVVDTLGDRFGINVADVGERGRLEARIDKVCFGAENR
2nd(r): SHHHHHHHHHHTT   GGGGS HHHHHHHHHHH  *****
2nd(s): OHHHHHHHHHHOOOOOHHHHOOHHHHHHHHHHHHOODDDDD
Switch: 00000000001000000000000000000011000000


>2VI7A

[0]
1st   : MTAESPTIRLERYSERHVEGLTALYNDPAVARQVLQMPYQSVEQRRKRLHDSADDDRLLI
2nd(r): ****** EEEEE  GGGHHHHHHHHTSHHHHTTSS  SS  HHHHHHHHTT *  TTEEE
2nd(s): DDDDDDOSSSSSOOHHHHHHHHHHHHOOHHHHOOOOOOOOOOHHHHHHHHHOOODOOOOSSS
Switch: 0000??0100000000000000000000000000000000000000011000000000

[60]
1st   : LVALHQGDVIGSASLEQHPRIRRSHSGSIGMGVAVAWQGKGVGSRLLGELLDIADNWMNL
2nd(r): EEEEETTEEEEEEEEEE SSGGGTTEEE TT  EESSTTTTHHHHHHHHHHHIIIIIS
2nd(s): SSSSSOOSSSSSSSSSSOOOHHHOOSSSOOOOOSSOOOOOOHHHHHHHHHHHHHHHHOOO
Switch: 00000000000000000000000000000000000000000000000000000000001000
```

```
[120]
1st   : RRVELTVYTDNAPALALYRKFGFETEGEMRDYAVRDGRFVDVYSMARLRRVEGRVGE
2nd(r): SEEEEEEETT HHHHHHHHHTT EEEEEEEEEEEETTEEEEEEEEEEE *******
2nd(s): OSSSSSSSOOOHHHHHHHHHOOOSSSSSSSSSSSSOOSSSSSSSSSSOODDDDDDD
Switch: 00000000000000000000000000000000000000000000000?0000000


>2WPWA

[0]
1st   : MNDTAGELEFVPLAANDDETVGQWLDLMALAAETGPRAAPPCNVDMVGSLRFAPPATALD
2nd(r): ***  SSEEEEE  TT HHHHHHHHHHHHHHHHTSSS     HHHHHHTTT   TTEEEE
2nd(s): DDDOOOOSSSSSOOOOOHHHHHHHHHHHHHHHHOOOOOOOOOHHHHHHOOOOOOOSSSS
Switch: 000???0100000000000000000000010000000000000000111000000000

[60]
1st   : DWVVRSGGRVVGALRLALPDGAPTARVDQLLVHPGRRRRGIGRALWAHARELARKHDRTT
2nd(r): EEEEEETTEEEEEEEEEESS SEEEEEEEEE TTS SSSHHHHHHHHHHHHHHHTT SE
2nd(s): SSSSSSOOSSSSSSSSSSOOOOSSSSSSSSSOOOOOOOOHHHHHHHHHHHHHHHOOOOS
Switch: 00000000100000000000000000000000111000000000000000000000000

[120]
1st   : LTATVVESLPSGPAQDPGPAAFAAAMGAHRSDIPAGTHQWLDLDRHDPLADGVPAVPAGY
2nd(r): EEEEEEE  SSS     HHHHHHHHHT EE SS  EEEEEEETTT  TTTT S    TTE
2nd(s): SSSSSSSOOOOOOOOOOHHHHHHHHHOOSSOOOOOSSSSSSSOOOOOOOOOOOOOOOOS
Switch: 00000000000000000000000010000000000000000000000000000000000

[180]
1st   : SLVTWGTITPDEYAVPVSELELSLGAGPVDRAAQEVRTSYARQFETMRVGRGRRAYHTGA
2nd(r): EEEEE SS  HHHHHHHHHTT ********  THHHHHHHHHHHHHHHHHTT EEEEEEE
2nd(s): SSSSSOOOOOHHHHHHHHHOOODDDDDDDDOOOHHHHHHHHHHHHHHHHHHOOOSSSSSSS
Switch: 00000000000000000010000000000000111111110000000000010000000

[240]
1st   : VHDATGALAGYTSVSKTTGNPAYALQGMTVVHREHRGHALGTLLKLANLEYVLRHEPEVR
2nd(r): EETTTTEEEEEEEEEE SS TTEEEEEEEEE GGG SSSHHHHHHHHHHHHHHHH TT
2nd(s): SSOOOOSSSSSSSSSSOOOOOOSSSSSSSSSOHHHOOOOHHHHHHHHHHHHHHHHOOOOO
Switch: 00000000000000001000000000111000000000011000000000000000000
```

```
[300]
1st   : LVETANAEDNHPMIAVNAALGFEPYDRWVFWTAEAGPSD
2nd(r): EEEEEEETT HHHHHHHHTTT EEEEEEEEEEEE
2nd(s): SSSSSSSOOOHHHHHHHHOOOOSSSSSSSSSSSOOOOO
Switch: 00000000000000000010010000000000000000?


>3FS8A

[0]
1st   : MPNNISKSAIIKEGVIIGENVTIEDNVYIDYGCIIRDNVHIKKGSFIGARSILGEYLVDF
2nd(r): ** EE TT EE TT EE SSEEE TT EE TT EE SSEEE TT EE TT EEEE  TTH
2nd(s): DDOSSOOOOSSOOOOSSOOOSSSOOOOSSOOOOSSOOOSSSOOOOSSOOOOSSSSOOOOH
Switch: 00000000000000000000100000000000000000000000000000000000110

[60]
1st   : YNDRINKKHPLIIGENALIRTENVIYGDTIIGDNFQTGHKVTIRENTKIGNNVKIGTLSD
2nd(r): HHHT      EEE TT EE TT EEESS EE TT EE SS EE SS EE SS EE TT E
2nd(s): HHHOOOOOOOSSSOOOOSSOOOOSSSOOOSSOOOOSSOOOOSSOOOOSSOOOOSSOOOOS
Switch: 00100000000000000000000000010000000000000000000000000000000

[120]
1st   : IQHHVYIGNYVNIHSNVFVGEKSIIKDFVWLFPHVVLTNDPTPPSNELLGVTIELFAVIA
2nd(r): E SS EE SS EE TT EE TT EE TT EE TT EE   SSSS S     EE TT EE
2nd(s): SOOOOSSOOOOSSOOOOSSOOOOSSOOOOSSOOOOSSOOOOOOOOOOOOOOSSOOOOSSO
Switch: 00000000000000000000000000000000000000000000000000000000000

[180]
1st   : ARSVVLPGIHINEDALVGAGAVVTKDVPKETVVVGNPAREICSIRKIKNKITGEQVYPWR
2nd(r): TT EE TT EE TT EE TT EE S B TTEEEEETTEEEEEEGGG B TTT  B  SGG
2nd(s): OOOSSOOOOSSOOOOSSOOOOSSOOOSOOOSSSSSOOSSSSSSHHHOSOOOOOOSOOOHH
Switch: 00000000000000000000000000000000010010000000000000000000000

[240]
1st   : YTFKRGMPWEETDYDTWIKNISIEN
2nd(r): GT  TTSTTTTS HHHHHHH ****
2nd(s): HOOOOOOOOOOOOHHHHHHHODDDD
Switch: 00000000000000000111?000
```

```
>3MQHA

[-2]
1st   : HMATIHPTAIVDEGARIGAHSRIWHWVHICGGAEIGEGCSLGQNVFVGNRVRIGNRVKIQ
2nd(r):    EE TT EE TT EE TT EE TT EE TT EE TT EE TT EE SS EE TT EE
2nd(s): OOOSSOOOOSSOOOOSSOOOOSSOOOOSSOOOOSSOOOOSSOOOOSSOOOOSSOOOOSSO
Switch: 0?01000000000000000000000000000000000000000000000000000000000

[59]
1st   : NNVSVYDNVFLEDDVFCGPSMVFTNVYNPRAAIERKSEYRDTIVRQGATLGANCTVVCGA
2nd(r): TT EE TTEEE TT EE TT B  S SS BTTB  GGG   EEE TT EE TT EE TT
2nd(s): OOOSSOOOSSSOOOOSSOOOOSOOOOOOOSOOSOOHHHOOOSSSOOOOSSOOOOSSOOOO
Switch: 00000000000000000000001000000000000000000000000000000000000

[119]
1st   : TIGRYAFVGAGAVVNKDVPDFALVVGVPARQIGWMSRHGEQLDLPLRGNAEATCPHTGER
2nd(r): EE TT EE TT EE S B TTEEEETTTTEEEEEB TTS B S  SSSSEEEE TTT  E
2nd(s): SSOOOOSSOOOOSSOOOSOOOSSSSOOOOSSSSSSOOOOOSOOOOOOOOSSSSOOOOOOS
Switch: 00000000000000000000000000000000000000000000000000000000000

[179]
1st   : YILTDGVCRLA
2nd(r): EEEETTEEEE
2nd(s): SSSSOOSSSSO
Switch: 00000000000

>3N37A

[0]
1st   : MKLSRISAINWNKISDDKDLEVWNRLTSNFWLPEKVPLSNDIPAWQTLTVVEQQLTMRVF
2nd(r): ****      TTS S HHHHHHHHHHHHT   GGGS GGGGHHHHTTS HHHHHHHHHHH
2nd(s): DDDDOOOOOOOOOOOOHHHHHHHHHHHHHOOOOHHHOOHHHHHHHHOOOOHHHHHHHHHHH
Switch: 0?????00000000000000000001100001110011110000110000000000000

[60]
1st   : TGLTLLDTLQNVIGAPSLMPDALTPHEEAVLSNISFMEAVHARSYSSIFSTLCQTKDVDA
2nd(r): HHHHHHHHHIIIIIHHHHGGG SSHHHHHHHHHHHHHHHHHHHHHHHHHHS HHHHHH
2nd(s): HHHHHHHHHHHHHHHHHHHHHOOOHHHHHHHHHHHHHHHHHHHHHHHHHHHOOHHHHHH
Switch: 00000000000000100111100000000000000000000000000111100000000
```

```
[120]
1st   : AYAWSEENAPLQRKAQIIQQHYRGDDPLKKKIASVFLESFLFYSGFWLPMYFSSRGKLTN
2nd(r): HHHHHHH HHHHHHHHHHHHHHHSS HHHHHHHHHHIIIIITHHHHHHHHHHHHTT SHH
2nd(s): HHHHHHHOHHHHHHHHHHHHHHHHOOOHHHHHHHHHHHHHHHHOHHHHHHHHHHHHOOOOHH
Switch: 0000111000000000000011100000000000000011100111000000011000011

[180]
1st   : TADLIRLIIRDEAVHGYYIGYKYQKNMEKISLGQREELKSFAFDLLLELYDNELQYTDEL
2nd(r): HHHHHHHHHHHHHHHHHHHHHHHHHHHHTTS HHHHHHHHHHHHHHHHHHHHHHHHHHHHH
2nd(s): HHHHHHHHHHHHHHHHHHHHHHHHHHHHOOOOHHHHHHHHHHHHHHHHHHHHHHHHHHHHH
Switch: 1000000000000000000000000011100110000000000000100000000000011

[240]
1st   : YAETPWADDVKAFLCYNANKALMNLGYEPLFPAEMAEVNPAILAALSPNADENHDFFSGS
2nd(r): STTSS HHHHHHHHHHHHHHHHHTT    S GGG    HHHHHHH  ***********
2nd(s): OOOOOOHHHHHHHHHHHHHHHHHHHOOOOOOOOHHHOOOOHHHHHHHOODDDDDDDDDDDD
Switch: 1111001100000000000001110000000111100000000011???00000000000

[300]
1st   : GSSYVMGKAVETEDEDWNF
2nd(r): ********************
2nd(s): DDDDDDDDDDDDDDDDDD
Switch: 00000000??????????0


>3NE7A

[-6]
1st   : MSIEIRKLSIEDLETLIEVARESWKWTYAGIYSEEYIESWIREKYSKEKLLNEIVRSQSN
2nd(r):   EEEEE  GGGHHHHHHHHHHHHHHHTTTTS HHHHHHHHHHHS HHHHHHHHHHHHTT
2nd(s): OOSSSSSOOHHHHHHHHHHHHHHHHHHHOOOOOOHHHHHHHHHHHOOHHHHHHHHHHHHOO
Switch: ??100000000000000000000000010000000000000001000000000000010

[60]
1st   : LDILFLGAFADSTLIGFIELKIIANKAELLRLYLKPEYTHKKIGKTLLLEAEKIMKKKGI
2nd(r): SSEEEEEEEETTEEEEEEEEEETTEEEEEEEEE GGGTTSSHHHHHHHHHHHHHHTT
2nd(s): OOSSSSSSSSOOSSSSSSSSSSSOOSSSSSSSSSOHHHOOOOHHHHHHHHHHHHHHOOO
Switch: 000000000000000000000000000000000000000011000000000000000100
```

```
[120]
1st   : LECRLYVHRQNSVGFSFYYKNGFKVEDTDGSDFIMEKKYES
2nd(r):  EEEEEEETT HHHHHHHHTTT EEEEEETTEEEEEEE **
2nd(s): OSSSSSSSOOOHHHHHHHHOOOOSSSSSSOOSSSSSSSODD
Switch: 00000000000000000001000000011000000000000
```

```
>3QB8A

[0]
1st   : MYTLIKLTSEYTSRAISFTSRNFVASEPTSIALKLTTCDFTTSFQNIMKQCVDYGHSFAF
2nd(r):   EEEE  GGGHHHHHHHHHHHHHHH HHHHHTT  HHHHHHHHHHHHHHHHHTT  EEE
2nd(s): OOSSSSOOHHHHHHHHHHHHHHHHHHHHOHHHHHOOOOHHHHHHHHHHHHHHHHHOOOOSSS
Switch: 00000000000000000000000000000000000000000000000000000000000000

[60]
1st   : VDADDNIKAQILNIPYDAYENMHYGNIRETDPMFDLFGNLDSYTPDDKCLYVFAIGSEVT
2nd(r): E TT  EEEEEEEEEHHHHHT      GGGHHHHHHHHGGGGS  SS EEEEEEEEESS
2nd(s): SOOOOOSSSSSSSSSHHHHHOOOOOOOHHHHHHHHHHHHHHHHOOOOOOSSSSSSSSSOOO
Switch: 00000000000000000000000000000000000000000000000000000000000000

[120]
1st   : GKGLATKLLKKTIEESSSHGFKYIYGDCTNIISQNMFEKHGFETVGSVKYKGYQYGITKP
2nd(r): SSSHHHHHHHHHHHHHHHTT  EEEEEE SHHHHHHHHHTT EEEEEEESTT  BTTB T
2nd(s): OOOHHHHHHHHHHHHHHHOOOOSSSSSSOOHHHHHHHHHOOOSSSSSSSOOOOOSOOSOO
Switch: 00000000000000000000000000000000000000000000000000000000000000

[180]
1st   : FDSINCTEYIKRMVKTI
2nd(r): TTT  S SEEEEEEEE
2nd(s): OOOOOOOOSSSSSSSSO
Switch: 00000000000000000
```

```
>3SMAA

[0]
1st   : MIRHIDARREDLEPDRQDRELVTRDRLASDLAALGVRPGGVLLVHASLSALGWVCGGAQA
2nd(r): ******************  EE HHHHHHHHHHHT  TT EEEEEE STTS EETTHHHH
2nd(s): DDDDDDDDDDDDDDDDDDOOSSOHHHHHHHHHHHHOOOOOOSSSSSSOOOOOOSSOOHHHH
Switch: 0000000000000?????00000000000000000000000000000111000000000
```

```
[60]
1st   : VVLALQDAVGKEGTLVMPTFSGDLSDPSTWRRPPVPEDWWPVIREQMPPFDPDLTPTRGM
2nd(r): HHHHHHHHH TT EEEEE   TTSS GGG  SS   GGGHHHHHHH     TTT   SSS
2nd(s): HHHHHHHHHOOOOSSSSSOOOOOOOOHHHOOOOOOOHHHHHHHHHHOOOOOOOOOOOOOO
Switch: 00000000000000000000000000000000000000000000000000000000000

[120]
1st   : GAVAECFRRAAGAVRSGHPQNSFAAWGAHAEQVVAEHGLTERLGRGSPLEQVYRLDGQVL
2nd(r):  HHHHHHTTSTT EE S TTT EEEEETTHHHHHTT  STTTTSTTSHHHHHHHTT EEE
2nd(s): OHHHHHHOOOOOOSSOOOOOOOSSSSSOOHHHHHOOOOOOOOOOOOOHHHHHHHOOOSSS
Switch: 00000000000000000000000000000000000000000000000000000000000

[180]
1st   : LLGCGFESNTSFHLAEYRTAYPGRRSHRRRVPVPEGDRVRWVEQEDIVYFEEDFQTMGES
2nd(r): EES  GGG TTHHHHHHH   TT  EEEEEEEEEETTEEEEEEEEE    TTHHHHHHH
2nd(s): SSOOOHHHOOOHHHHHHHOOOOOOOSSSSSSSSSSOOSSSSSSSSSSOOOOOOHHHHHHH
Switch: 00000000001000000000000000000000000000000000000000000000000

[240]
1st   : CLTRTPGHSRGTVGEAAAVLYGQRAFVDLACEWMTAHRDLARAVGA
2nd(r): HHHHSTT EEEEETTEEEEEEEHHHHHHHHHHHHHHH    *****
2nd(s): HHHHOOOOSSSSSOOSSSSSSSHHHHHHHHHHHHHHHHOOOODDDDD
Switch: 00010000000000000000000000000000000000??0000


>3TFYA

[0]
1st   : MKGSRIELGDVTPHNIKQLKRLNQVIFPVSYNDKFYKDVLEVGELAKLAYFNDIAVGAVC
2nd(r):   S SEEEEE  TTTHHHHHHHHHHH SS   HHHHHHHTTSGGGEEEEEETTEEEEEEE
2nd(s): OOOOOSSSSSOOOOOHHHHHHHHHHHHOOOOOOHHHHHHHOOOHHHSSSSSSOOSSSSSSS
Switch: ???000000000000000000000000000000000011111100000001000000

[60]
1st   : CRVDHSQNQKRLYIMTLGCLAPYRRLGIGTKMLNHVLNICEKDGTFDNIYLHVQISNESA
2nd(r): EEEEEETTEEEEEEEEEEE GGG SSSHHHHHHHHHHHHHHHH   SEEEEEEETT HHH
2nd(s): SSSSSSOOSSSSSSSSSSSOHHHOOOOHHHHHHHHHHHHHHHHOOOOSSSSSSSOOOHHH
Switch: 00001100110000000000000000000000000000011100000000000000000
```

```
[120]
1st   : IDFYRKFGFEIIETKKNYYKRIEPADAHVLQKNLKVPSGQNADVQKTDN
2nd(r): HHHHHHTT EEEEEESS SSSSSS  EEEEEEE  **************
2nd(s): HHHHHHOOOSSSSSSOOOOOOOOOOOSSSSSSSOODDDDDDDDDDDDD
Switch: 000001000000000000000000000000000??????????????


>3W6SA

[0]
1st   : MDAESIEWKLTANLRNGPTFFQPLADSIEPLQFKLIGSDTVATAFPVFDTKYIPDSLINY
2nd(r): ****  GGGBGGG  S  SS   SSSB   EEEE TTS  EEEEEEESSGGGS HHHHHH
2nd(s): DDDDOOHHHSHHHOOOOOOOOOOOOOOSOOOSSSSOOOOOOSSSSSSSOOHHHOOHHHHHH
Switch: ?????000000000000000000010000000000000000000000000000000000

[60]
1st   : LFKLFNLEIESGKTYPQLHSLTKQGFLNYWFHSFAVVVLQTDEKFIQDNQDWNSVLLGTF
2nd(r): HHHHHHHHHHHTSSSS  S   HHHHHHHHTSSEEEEEES S SS  SS  HHHHEEEEE
2nd(s): HHHHHHHHHHHOOOOOOOOOOOOHHHHHHHHOOOSSSSSSOOOOOOOOOOOOHHHHSSSSS
Switch: 000000000010000000000000000000000000010000000000000000000

[120]
1st   : YIKPNYAPRCSHNCNAGFLVNGAHRGQKVGYRLAQVYLNWAPLLGYKYSIFNLVFVTNQA
2nd(r): EEEESSSGGGTTEEEEEEEE GGGTTS HHHHHHHHHHHHTGGGT  EEEEEEEETT TH
2nd(s): SSSSOOOHHHOOSSSSSSSSOHHHOOOOHHHHHHHHHHHHOHHHOOOSSSSSSSOOOOH
Switch: 000000000000000000000000000000000000000010000000000000000011

[180]
1st   : SWKIWDKLNFQRIGLVPHAGILNGFSEPVDAIIYGKDLTKIEPEFLSME
2nd(r): IIIIITTTT EEEEEEEEEE  TT SS EEEEEEEEETTS  HHHH
2nd(s): HHHHHOOOOOSSSSSSSSSSOOOOOOOOSSSSSSSSOOOOOHHHHOOO
Switch: 11?1111100000000000000000000000000000000000000000?


>4AVAA

[0]
1st   : MDGIAELTGARVEDLAGMDVFQGCPAEGLVSLAASVQPLRAAAGQVLLRQGEPAVSFLLI
2nd(r): *       S  HHHHTTSGGGTT  HHHHHHHHHH EEEEE TT EEE TTSB   EEEE
2nd(s): DOOOOOOOOOOHHHHOOOHHHOOOOHHHHHHHHHHOSSSSSOOOOSSSOOOOSOOOSSSS
Switch: 0???????000000010011100000001000000000000000000000010010000
```

```
[60]
1st   : SSGSAEVSHVGDDGVAIIARALPGMIVGEIALLRDSPRSATVTTIEPLTGWTGGRGAFAT
2nd(r): EE  EEEEEE TT  EEEEEE TT EESHHHHHHT B SSEEEESS EEEEEE HHHHHH
2nd(s): SSOOSSSSSSOOOOOSSSSSSOOOOSSOHHHHHHOOSOOOSSSSOOOSSSSSSOHHHHHH
Switch: 00110000000000000000000000010000000100000001110000001000000

[120]
1st   : MVHIPGVGERLLRTARQRLAAFVSPIPVRLADGTQLMLRPVLPGDRERTVHGHIQFSGET
2nd(r): HHHSTTHHHHHHHHHHHHHHH   EEEE TT  EEEEEE  TT GGGT   SS   HHH
2nd(s): HHHOOOHHHHHHHHHHHHHHHHOOOSSSSOOOOOSSSSSSOOOOOHHHOOOOOOOOOHHH
Switch: 00100000000000000000110000000000000000000000010001110000000100

[180]
1st   : LYRRFMSARVPSPALMHYLSEVDYVDHFVWVVTDGSDPVADARFVRDETDPTVAEIAFTV
2nd(r): HHGGG ***** HHHHHHHHHH  SSEEEEEEEETTEEEEEEEEEE SS TTEEEEEEEE
2nd(s): HHHHHODDDDDOHHHHHHHHHHOOOOSSSSSSSSOOSSSSSSSSSSOOOOOOSSSSSSSS
Switch: 000000?????000000000110000000000010010000000000000000000000

[240]
1st   : ADAYQGRGIGSFLIGALSVAARVDGVERFAARMLSDNVPMRTIMDRYGAVWQREDVGVIT
2nd(r):  GGGTTSSHHHHHHHHHHHHHHHTT  EEEEEEETT HHHHHHHHTTT   EE STTEEE
2nd(s): OHHHOOOOHHHHHHHHHHHHHHHOOOOSSSSSSSOOOHHHHHHHHOOOOOOSSOOOOSSS
Switch: 000000000000000000000001000000000000000000000100000001100000

[300]
1st   : TMIDVPGPGELSLGREMVDQINRVARQVIEAVG
2nd(r): EEEE   TTTSSS HHHHHHHHHHHHIIIII
2nd(s): SSSSOOOOOOOOOOHHHHHHHHHHHHHHHHHOO
Switch: 00000001110000100000000000000110?


>4EABA

[0]
1st   : MSASLAIGGVVIIGGGGHAKVVIESLRACGETVAAIVDADPTRRAVLGVPVVGDDLALPM
2nd(r): **    TT EEEE  SHHHHHHHHHHHHTT  EEEEE SS  * EETTEEEEESGGGHHH
2nd(s): DDOOOOOOOSSSSOOOHHHHHHHHHHHHHOOOOSSSSSOOOOODOSSOOSSSSSOHHHHHH
Switch: 00000000000000000000000000000000000000000?0?1000010000000000
```

```
[60]
1st   : LREQGLSRLFVAIGDNRLRQKLGRKARDHGFSLVNAIHPSAVVSPSVRLGEGVAVMAGVA
2nd(r): HHHTT  EEEE    HHHHHHHHHHHHTT EE  EE TT EE TT EE SS EE TT E
2nd(s): HHHOOOOSSSSOOOOHHHHHHHHHHHHHOOOSSOOSSOOOOSSOOOOSSOOOOSSOOOOS
Switch: 00000000000000000000000000000000000000000000000000000000000

[120]
1st   : INADSWIGDLAIINTGAVVDHDCRLGAACHLGPASALAGGVSVGERAFLGVGARVIPGVT
2nd(r): E TT EE TT EE TT EE TT EE TT EE TT EE TT EE TT EE TT EE TT E
2nd(s): SOOOOSSOOOOSSOOOOSSOOOOSSOOOOSSOOOOSSOOOOSSOOOOSSOOOOSSOOOOS
Switch: 00000000000000000000000000000000000000000000000000000000000

[180]
1st   : IGADTIVGAGGVVVRDLPDSVLAIGVPAKIKGDRS
2nd(r): E TT EE TT EE S B TT EEETTTTEE   **
2nd(s): SOOOOSSOOOOSSOOOSOOOOSSSOOOOSSOOODD
Switch: 00000000000000000000000000000000?00


>4FD4A

[0]
1st   : MVAPESIVLRVARLDELEQVREILHRIYYPEEGITISYVHGKSHTLDDERFSLSFVEQGT
2nd(r): ***** EEEEE  GGGHHHHHHHIIIIITTT HHHHHBTT SS  HHHHHHHHTTTTTT
2nd(s): DDDDDOSSSSSSOOHHHHHHHHHHHHHHHHOOOOHHHHHSOOOOOOOOHHHHHHHHOOOOOOO
Switch: ?????100000000000000000000000000000100000000000000000011100

[60]
1st   : VVVAEDSAAKKFIGVSIAGPIQPGDPDAMVEEAATTETKKWGDILKLLALLERTADVCGR
2nd(r): EEEEEETTTTEEEEEEEEEEE TTHHHHHHHHHHHSS HHHHHHHHHHHHHHHHH HHHH
2nd(s): SSSSSSOOOOSSSSSSSSSSOOOHHHHHHHHHHHHOOOHHHHHHHHHHHHHHHHHOHHHH
Switch: 00000000000000000000000000000001100000000000000000000000000

[120]
1st   : YGLEKAYHVHILAVDPTYRGHSLGQRLLQFQMDLSKKLGFKAISGDFTSVFSVKLAEKLG
2nd(r): HT S EEEEEEEEE TTS SS HHHHHHHHHHHHHHHHT SEEEEEE SHHHHHHHHHTT
2nd(s): HOOOOSSSSSSSSSOOOOOOOOHHHHHHHHHHHHHHHHOOOSSSSSSOOHHHHHHHHHOO
Switch: 00000000000000011100000000000000000001000000000000000000000
```

```
[180]
1st   : MECISQLALGDYRDEKGEKLFEPLDVHQVIKTCVKLL
2nd(r):  EEEEEEEGGG   TT    B  SSSS EEEEEEEE
2nd(s): OSSSSSSSHHHOOOOOOOOOSOOOOOOOSSSSSSSSO
Switch: 00000000111010000010000011100000000000
```

```
>4FD5A
```

```
[0]
1st   : MLDSKLNNIRFETISSKYYDDVIEHLRQTFFADEPLNKAVNLTRPGQGHPLLEQHSLSTL
2nd(r): ******   EEEE  GGGHHHHHHHHHHHTTTTSHHHHHTT   TTT  HHHHHHHHHHH
2nd(s): DDDDDDOOOSSSSOOHHHHHHHHHHHHHHHOOOOOHHHHHOOOOOOOOOOHHHHHHHHHHH
Switch: 0000??00000000000000000000001000000000000000000000000000000
```

```
[60]
1st   : KDNVSIMAISNDGDIAGVALNGILYGNTDIEKSREKLNEIQDESFKKIFKLLYEQNLKIN
2nd(r): TTS  EEEE TTS EEEEEEEEEEETTS TTHHHHHHHH   HHHHHHHHHHHHHHTT
2nd(s): OOOOOSSSSOOOOOSSSSSSSSSSSOOOOOOHHHHHHHHOOOHHHHHHHHHHHHHHOOOO
Switch: 00000000000000000000000000000010000001100000000000000000000
```

```
[120]
1st   : LFKQFDVDKIFEIRILSVDSRFRGKGLAKKLIEKSEELALDRGFQVMKTDATGAFSQRVV
2nd(r): HHHHHT SEEEEEEEEEE GGGTTSSHHHHHHHHHHHHHHHTT  EEEEEE SHHHHHHH
2nd(s): HHHHHOOOSSSSSSSSSSOHHHOOOOHHHHHHHHHHHHHHHOOOOSSSSSSOOHHHHHHH
Switch: 00000000000000000000000000000000000000000000000000000000000
```

```
[180]
1st   : SSLGFITKCEINYTDYLDENGEQIFVVDPPHEKLKIMCKVIN
2nd(r): HHTT EEEEEEEGGG B TTSSBS    TT  EEEEEEEE
2nd(s): HHOOOSSSSSSSHHHOSOOOOOSOOOOOOOOOSSSSSSSSOO
Switch: 00000000000000000000000000000000000000000
```

```
>4FD7A
```

```
[0]
1st   : MKWTRSVKVPFPSVWHRFQAKDLTSQQLVWYRVQDLPEDRFEDAIRHMCDYFARDELMNQ
2nd(r): *     TTS SS EEEEEEEE SSSS EEEEEEEE  GGGHHHHHHHIIIIIHHHSHHHH
2nd(s): DOOOOOOOOOOOOSSSSSSSSSOOOOOOSSSSSSSSOOHHHHHHHHHHHHHHHHHHOHHHH
Switch: 00000000000000000000000000000000000000000000000000000000000
```

```
[60]
1st   : AKGLAKDLVAMGDVVALWKAMLPDRMSLVCFREGSDEIVGVNILDVASRSDKDNAQFNSA
2nd(r): HHTGGG HHHHHHHHHHHHHHGGGS  EEEEETT  SEEEEEEEEEEETT       S H
2nd(s): HHOHHHOHHHHHHHHHHHHHHHHHOOOSSSSSOOOOOSSSSSSSSSSOOOOOOOOOOOH
Switch: 000111000000000000000000000000000000000000000000000000000000

[120]
1st   : IFQAIYDTIEYVSHQANIFDRYNVDHYLNAMGLSVDPKYRGRGIATEILRARIPLCRAVG
2nd(r): HHHHHHHHHHHHHHHHHTHHHHHT SEEEEEEEEEE GGGTTSSHHHHHHHTHHHHHHHHT
2nd(s): HHHHHHHHHHHHHHHHHOHHHHHOOOSSSSSSSSSSOHHHOOOOHHHHHHHOHHHHHHHHO
Switch: 000000000000000100000100000000000000000000000000000000000000

[180]
1st   : LKLSATCFTGPNSQTAATRVGFQEDFTITYGELARVDQRFNYPGIEENFCKYMSLRVD
2nd(r):   EEEEEE SHHHHHHHHHHT EEEEEEEHHHHHHH TT   TT TTSEEEEEEEE
2nd(s): OOSSSSSSOOHHHHHHHHHHOOSSSSSSSHHHHHHHOOOOOOOOOOOOSSSSSSSSOO
Switch: 000000000000000000000000000000000000111000000000000000000


>4HNYA

[0]
1st   : MSRKRSTKPKPAAKIALKKENDQFLEALKLYEGKQYKKSLKLLDAILKKDGSHVDSLALK
2nd(r): ************************************************** HHHHHH
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDOHHHHHH
Switch: 0000000000??????????????????????????????????????????1100000

[60]
1st   : GLDLYSVGEKDDAASYVANAIRKIEGASASPICCHVLGIYMRNTKEYKESIKWFTAALNN
2nd(r): HHHHHHHT HHHHHHHHHHHT ******  HHHHHHHHHHHHHTT HHHHHHHHHHHHHT
2nd(s): HHHHHHHOOHHHHHHHHHHHOODDDDDDOOHHHHHHHHHHHHHHOOOHHHHHHHHHHHHO
Switch: 00100110010000000111117777777000011110000110001000000000010

[120]
1st   : GSTNKQIYRDLATLQSQIGDFKNALVSRKKYWEAFLGYRANWTSLAVAQDVNGERQQAIN
2nd(r): T   THHHHHHHHHHHHTT HHHHHHHHHHHHHH TT HHHHHHHHHHHHTT HHHHHH
2nd(s): OOOOOHHHHHHHHHHHHOOOHHHHHHHHHHHHHHOOOOHHHHHHHHHHHHHOOOHHHHHH
Switch: 000001000011111111001000000001111100001111111110000100100001
```

```
[180]
1st   : TLSQFEKLAEGKISDSEKYEHSECLMYKNDIMYKAASDNQDKLQNVLKHLNDIEPCVFDK
2nd(r): HHHHHHHHT S   GGGHHHHHHHHHHHHHHHHHHTT HHHHHHHHHHHHHHGGG   H
2nd(s): HHHHHHHHOOOOOOHHHHHHHHHHHHHHHHHHHHHHOOOHHHHHHHHHHHHHHHHHOOOH
Switch: 1111111110??00111111111111000001111100011110000000111110001

[240]
1st   : FGLLERKATIYMKLGQLKDASIVYRTLIKRNPDNFKYYKLLEVSLGIQGDNKLKKALYGK
2nd(r): HHHHHHHHHHHHHTT HHHHHHHHHHHHHH TT HHHHHHHHHHT TT HHHHHHHHHH
2nd(s): HHHHHHHHHHHHHOOOHHHHHHHHHHHHHHHOOOOHHHHHHHHHHHOOOOOHHHHHHHHHH
Switch: 11111111111111001111111000001100001000010000100000000100100

[300]
1st   : LEQFYPRCEPPKFIPLTFLQDKEELSKKLREYVLPQLERGVPATFSNVKPLYQRRKSKVS
2nd(r): HHHH TT HHHHHHHHHH   HHHHHHHHHHHHHHHHHTT TTHHHHHHHHHHHHHHHHH
2nd(s): HHHHOOOOHHHHHHHHHHOOOHHHHHHHHHHHHHHHHHHOOOOOHHHHHHHHHHHHHHHH
Switch: 11110000111110001100011100000011111111100111111111111111100

[360]
1st   : PLLEKIVLDYLSGLDPTQDPIPFIWTNYYLSQHFLFLKDFPKAQEYIDAALDHTPTLVEF
2nd(r): HHHHHHHHHHHHT  TTTSHHHHHHHHHHHHHHHHHTT HHHHHHHHHHHHHH TT HHH
2nd(s): HHHHHHHHHHHHOOOOOOOHHHHHHHHHHHHHHHHHOOOHHHHHHHHHHHHHHOOOOHHH
Switch: 00000110111100000001111111111111111100000011000000111000011

[420]
1st   : YILKARILKHLGLMDTAAGILEEGRQLDLQDRFINCKTVKYFLRANNIDKAVEVASLFTK
2nd(r): HHHHHHHHHHTT HHHHHHHHHHHTT TT HHHHHHHHHHHHTT HHHHHHHTSTTT
2nd(s): HHHHHHHHHHOOOHHHHHHHHHHHHOOOOOOHHHHHHHHHHHHHHOOOHHHHHHHOOOOO
Switch: 00000011111000000100000001110001111110000111000111110001111

[480]
1st   : NDDSVNGIKDLHLVEASWFIVEQAEAYYRLYLDRKKKLDDLASLKKEVESDKSEQIANDI
2nd(r): BTTBBTTBSSGGGTS HHHHHHHHHHHHHHHHHHHHHHHHH ********** HHHHH
2nd(s): SOOSSOOSOOHHHOOOHHHHHHHHHHHHHHHHHHHHHHHHHHODDDDDDDDDDDOHHHHH
Switch: 111111?11111100011111111111111111111111111???00?????111110

[540]
1st   : KENQWLVRKYKGLALKRFNAIPKFYKQFEDDQLDFHSYCMRKGTPRAYLEMLEWGKALYT
2nd(r): HHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHTTTHHHHHHHHT HHHHHHHHHHTTGGG
2nd(s): HHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHOOOHHHHHHHHOOHHHHHHHHHHOOHHH
Switch: 000110000000000000100000000001111111111110011101110000011011
```

```
[600]
1st   : KPMYVRAMKEASKLYFQMHDDRLKRKSDSLDENSDEIQNNGQNSSSQKKKAKKEAAAMNK
2nd(r): SHHHHHHHHHHHHHHHHHHHHHHHHHHHTTT  **************************
2nd(s): OHHHHHHHHHHHHHHHHHHHHHHHHHHHOOOOODDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 000011110000000111111111?????????000000000000?????????????

[660]
1st   : RKETEAKSVAAYPSDQDNDVFGEKLIETSTPMEDFATEFYNNYSMQVREDERDYILDFEF
2nd(r): ****************** TT HHHHT S HHHHHIIIIIHHHHHH  TTT  HHHHHHH
2nd(s): DDDDDDDDDDDDDDDDDDOOOOHHHHOOOOHHHHHHHHHHHHHHHHHOOOOOOOHHHHHHH
Switch: ????????????????????000011111000111100001000111100111001111111

[720]
1st   : NYRIGKLALCFASLNKFAKRFGTTSGLFGSMAIVLLHATRNDTPFDPILKKVVTKSLEKE
2nd(r): HHHTT HHHHHHHHHHHHHHH SSSHHHHHHHHHHHHHT ***   HHHHHHHHHHHGGG
2nd(s): HHHOOOHHHHHHHHHHHHHHHOOOOHHHHHHHHHHHHHHOODDDOOOHHHHHHHHHHHHHH
Switch: 111100100000001110001000010000000111111????111???111??11111

[780]
1st   : YSENFPLNEISNNSFDWLNFYQEKFGKNDINGLLFLYRYRDDVPIGSSNLKEMIISSLSP
2nd(r): S  ***********  HHHHHHHHT S  HHHHHHHHHTTTTTT  HHHHHHHHHHTTT
2nd(s): OOODDDDDDDDDDOOHHHHHHHHOOOOOHHHHHHHHHOOOOOOOOHHHHHHHHHHOOO
Switch: 1?????????????111111111??000000001100000?010001000111000

[840]
1st   : LEPHSQNEILQYYLYPYDVPDY
2nd(r): S HHHHHHHHHHTGGGTS
2nd(s): OOHHHHHHHHHHHOHHHOOOOO
Switch: 00000011111117?11000000


>4J3GA

[0]
1st   : MTLLIRHATEADLPALLAIYNDAVENTLAIWNETLVDLENRHQWLENRNRDGFPVLVAER
2nd(r):    EEEE  GGGHHHHHHHHHHHHHH SSS       HHHHHHHHHHHHHT  EEEEEE
2nd(s): OOOSSSSOOHHHHHHHHHHHHHHHHHHOOOOOOOOOOOHHHHHHHHHHHHHHOOOSSSSSS
Switch: ??000000000000000000000000000000000000000000000001000000000
```

```
[60]
1st   : EGQVVGYASYGPFRPFEGFRHSSELSVYVASNARGGGIGRTLLAELIEEARERKVHVLIA
2nd(r): TTEEEEEEEEEESSSSGGGTTEEEEEEEE GGGTTSSHHHHHHHHHHHHHHTT  EEEE
2nd(s): OOSSSSSSSSSSOOOOHHHOOSSSSSSSSOHHHOOOOHHHHHHHHHHHHHHHOOOOSSSS
Switch: 00000000000000000000000000000011100000000000000000000000000

[120]
1st   : GIEAGNAASIALHRSQGFEECGTLKQVGQKFGRWLDLLFMQKIL
2nd(r): EEETT HHHHHHHHHTT EEEEEEEEEEEETTEEEEEEEEEEE
2nd(s): SSSOOOHHHHHHHHHOOOSSSSSSSSSSSSOOSSSSSSSSSSO
Switch: 00000000000001000000000000000000000000000


>4JJXA

[-2]
1st   : AMNSQLTLRALERGDLRFIHNLNNNRNIMSYWFEEPYESFDELEELYNKHIHDNAERRFV
2nd(r):  GGGG EEEE  GGGHHHHHTTTTTT S   SSS    SHHHHHHHHHTTTT SSEEEEE
2nd(s): OHHHHOSSSSOOHHHHHHHHHOOOOOOOOOOOOOOOOOOOHHHHHHHHHOOOOOOOSSSSS
Switch: 11111100000011100000111111111110011100000000001111100011100

[59]
1st   : VEDAQKNLIGLVELIEINYIHRSAEFQIIIAPEHQGKGFARTLINRALDYSFTILNLHKI
2nd(r): EE TT  EEEEEEEEEEETTTTEEEEEEEE GGGGGG  HHHHHHHHHHHHHTS  SEE
2nd(s): SSOOOOOSSSSSSSSSSOOOOSSSSSSSSOHHHHHHOOHHHHHHHHHHHHHHOOOOOSS
Switch: 00100001100000011100001100000001111110111000000000011100000

[119]
1st   : YLHVAVENPKAVHLYEECGFVEEGHLVEEFFINGRYQDVKRMYILQSKYLNRSE
2nd(r): EEEEETT HHHHHHHHHTT EEEEEEEEEEEETTEEEEEEEEEEEHHHHH  **
2nd(s): SSSSSOOOHHHHHHHHHOOOSSSSSSSSSSSSOOSSSSSSSSSSSHHHHHOODD
Switch: 00000000111000001100000000000001001000000000?11111???


>4KVOA

[0]
1st   : MAKVQLSPKEITLFRTALKCYETKQYKKGLKAIEPLLERHPEHGESLAIKGILLHSLGNT
2nd(r): ****   HHHHHHHHHHHHHHHTS THHHHHHHHHHHSS TT HHHHHHHHHHHHTS S
2nd(s): DDDDOOOHHHHHHHHHHHHHHHHOOOOHHHHHHHHHHHHOOOOOOHHHHHHHHHHHHHOOOO
Switch: ????000111011100000000001000001100011000000000000000001000
```

```
[60]
1st   : KEGYDNVRLGLRNDVGSGVCWHIFGLISRADKDYVQAAKCYINAHKLEKNNSSLLRDLAL
2nd(r): HHHHHHHHHHHHH TT HHHHHHHHHHHHTT HHHHHHHHHHHHH TT HHHHHHHHH
2nd(s): HHHHHHHHHHHHHOOOOHHHHHHHHHHHHHOOOHHHHHHHHHHHHHOOOOHHHHHHHHH
Switch: 10000000001110000100000000000000000000000000010000000000000

[120]
1st   : LQSQLRQYKALADTRNALLQDNPGVRANWSALAVAQFLRGEYASAYKIVDAFESTINQGV
2nd(r): HHHHTT HHHHHHHHHHHHH TTSHHHHHHHHHHHHHTT HHHHHHHHHHHHT SS S
2nd(s): HHHHOOOHHHHHHHHHHHHHHOOOOHHHHHHHHHHHHHOOOHHHHHHHHHHHHHOOOOOO
Switch: 00001000000000000000000000000000000010000000000000000000000

[180]
1st   : PVDTQEESEAMLFMNLVILKKDGVEDAYKHLLSIEKKVLDRVAFLETRAEYELYLSKMEE
2nd(r):  S SHHHHHHHHHHHHHHHHHTHHHHHHHHHHSGGG   HHHHHHHHHHHHHTT HHH
2nd(s): OOOOHHHHHHHHHHHHHHHHHOHHHHHHHHHHHOHHHOOOHHHHHHHHHHHHHOOOHHH
Switch: 00000000000000000000100000000001111000000000000000000000000

[240]
1st   : AKSTIYLLLDRNPDNHQYYYNLQRAYGYEDASGKVLDSAEWLNLYSQLAKRYPKSECPTR
2nd(r): HHHHHHHHHHH TT HHHHHHHHHHTTSS SSS  S HHHHHHHHHHTTTS TT SHHHH
2nd(s): HHHHHHHHHHHOOOOHHHHHHHHHHOOOOOOOOOOOOHHHHHHHHHHOOOOOOOOOHHHH
Switch: 00000000000000010000000000000000000000000000000000000000000

[300]
1st   : LPLEKLEGDEFLTHVDLYLRKKLKRGIPSVFVDVKSLYKDTKKCKVVEDLVSKYASSLST
2nd(r): THHHH  THHHHHHHHHHHHHHHHT TTHHHHHGGGGGGSHHHHHHHHHHHHHHTTTTT
2nd(s): OHHHHOOOHHHHHHHHHHHHHHHHHOOOOHHHHHHHHHHHHOHHHHHHHHHHHHHHOOOOO
Switch: 10000001110000000000000100000000000001010000000000000000000

[360]
1st   : TNKFSEDDDNSQIEIPTTLLWTYYFLAQHFDHVGELEKAEKYVDLAIDHTPTLVELFMTK
2nd(r): SSSSTTGGGSS    SSHHHHHHHHHHHHHHHHT SHHHHHHHHHHHHH TT HHHHHHH
2nd(s): OOOOOOHHHOOOOOOOOOHHHHHHHHHHHHHHHHHOOOHHHHHHHHHHHHHHOOOOHHHHHHH
Switch: 00000000010000000000000000000000000000000000000000000000000

[420]
1st   : ARISKHKGELQTAMEIMDHARKLDLQDRFINGKCAKYMLRNDENELAAKTVSLFTRNEAV
2nd(r): HHHHHHTT HHHHHHHHHHHHHH SS HHHHHHHHHHHHHTT HHHHHHHTTTS  SSS
2nd(s): HHHHHHOOOHHHHHHHHHHHHHHOOOOHHHHHHHHHHHHHOOOHHHHHHHOOOOOOOOO
Switch: 00000010000000000000001000000000000000000000000000000000000
```

```
[480]
1st   : GGAVGDLADMQCLWYMLEDGKSFARQKKFALALKRFSTVFKIFDTWADDQFDFHFFAFRK
2nd(r): SHHHHHHHHTT HHHHHHHHHHHHHTT HHHHHHHHHHHHHHHHHHHHTTTTHHHHHHHH
2nd(s): OHHHHHHHHOOOHHHHHHHHHHHHHOOOHHHHHHHHHHHHHHHHHHHHOOOOHHHHHHHH
Switch: 00000000000000000000000000000000000000000000000100000000000

[540]
1st   : GSLRTYLDLMSWEDSVYDDPSFREAAQGSIEIYFALFDLPFAKYSPKLPDFEKLSSGEIN
2nd(r): T HHHHHHHHHHHHTTT SHHHHHHHHHHHHHHHHHHH TTGGG   HHHHHHHHHT S
2nd(s): OOHHHHHHHHHHHHHOOOOOHHHHHHHHHHHHHHHHHHHHOOOHHHOOOHHHHHHHHHOOOO
Switch: 00000000000001000000000000000000000000000000000000000000000000

[600]
1st   : EEEEKKIYKKLKKDLSKRLERAEKLKEADKSRAKSEDGMPVKYDEDPLGENLVATSEPLK
2nd(r): HHHHHHHHHHHHHHHHHHHHHHHHHHHHHH  *********    S SSSTTTT S HHH
2nd(s): HHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHOODDDDDDDDDOOOOOOOOOOOOOOOOHHH
Switch: 00000000000000000000000000000000000000000000000011110000000

[660]
1st   : EAQKCLEKLLPYGDKNPSAYILAAQLYTRLKNFDTASKYLEQAKVILGQNDPTVISTEKF
2nd(r): HHHHHHTTTGGGTTT THHHHHHHHHHHHTT HHHHHHHHHHHHHSS SS HHHHHHHHH
2nd(s): HHHHHHOOOHHHOOOOOHHHHHHHHHHHHOOOHHHHHHHHHHHHHHOOOOOHHHHHHHHH
Switch: 00000010000000000000000000000000000000000000000000000000000

[720]
1st   : YNSIKTQSNAA
2nd(r): HHHHHTTSS
2nd(s): HHHHHOOOOOO
Switch: 00000000000


>4KVXA

[0]
1st   : MDIRPARISDLTGMQNCNLHNLPENYQLKYYLYHAISWPMLSYVATDPKGRVVGYVLAKM
2nd(r): * EEE  GGGHHHHHHTTTT GGGGTTHHHHHHHHHHTSTTS EEEE TTS EEEEEEEEE
2nd(s): DOSSSOOHHHHHHHHHOOOOOHHHHOOHHHHHHHHHOOOOOOSSSSOOOOOSSSSSSSSS
Switch: 00000000000000000000000000000000000000000000000000000000000000
```

```
[60]
1st   : EEEPKDGIPHGHITSVSVMRSYRHLGLAKRLMVQSQRAMVEVYGAKYMSLHVRKSNRAAI
2nd(r):  SS GGG   EEEEEEEE GGGTTSSHHHHHHHHHHHHHHHH  SEEEEEEETT HHHH
2nd(s): OOOOHHHOOOSSSSSSSSOHHHOOOOHHHHHHHHHHHHHHHHHOOOSSSSSSSOOOHHHH
Switch: 00000000010000000000000000000000000000000000000000000000000

[120]
1st   : HLYRDTLQFDVQGIESKYYADGEDAYAMHKDFSTLKFDTPETNDELAKTVQSLALNN
2nd(r): HIIIIIS  EEEEEETT STTS  EEEEEEE  **********************
2nd(s): HHHHHHOOOSSSSSSOOOOOOOOOSSSSSSSOODDDDDDDDDDDDDDDDDDDDDDD
Switch: 00000000000000000000000000000000000000000000000000000000000


>4PV6A

[0]
1st   : MVYMAINAVAGTIREFSPKDIESVYRIAQTSLTEYYTQALILDLHREWPESFMVYTVAGS
2nd(r): *****   SS EEEE  GGGHHHHHHHHHH SS   HHHHHHHHHHSGGG EEEEETTE
2nd(s): DDDDDOOOOOOSSSSOOHHHHHHHHHHHHHHHOOOOOOHHHHHHHHHHOHHHOSSSSSOOS
Switch: 00000???00110000000000000001100000011000001110111000001001

[60]
1st   : VVGFIVGSKYSRTEARILLFAVDERFRRMGVGSALMDAFLSLCREQNMLSVRLEVRTDND
2nd(r): EEEEEEEEESSSSEEEEEEEEE GGG SSSHHHHHHHHHHHHHHHTT  EEEEEEETT H
2nd(s): SSSSSSSSSOOOOSSSSSSSSSOHHHOOOOHHHHHHHHHHHHHHHHOOOOSSSSSSSOOOH
Switch: 00000000011000000000000111111010000000000000010000000000000

[120]
1st   : EAIRFYKKYGFVITAMLPNYYSDSSNAYTMWRIVLEHHH
2nd(r): HHHHHHHHTT EEEEEETT STT   EEEEEEES B
2nd(s): HHHHHHHHOOOSSSSSSOOOOOOOOOSSSSSSSOOSOOO
Switch: 00000000000000001000000000000000001000


>4R3KA

[0]
1st   : MELAEKDKGRDFTLRNARMDDIDQIIKINRLTLPENYPYYFFVEHLKEYGLAFFVAIVDN
2nd(r): **********  EEEE  GGGHHHHHHHHHH S    HHHHHHHHHHGGG EEEEETT
2nd(s): DDDDDDDDDDOOSSSSOOHHHHHHHHHHHHHHHOOOOOOHHHHHHHHHHHHHHOSSSSSOO
Switch: 00000000000000000011100000000000000000000000000001000000000000
```

```
[60]
1st   : SVVGYIMPRIEWGFSNIKQLPSLVRKGHVVSIAVLEEYRRKGIATTLLEASMKSMKNDYN
2nd(r): EEEEEEEEEEEEEE SSSSS  EEEEEEEEEEEE GGG SSSHHHHHHHHHHHHHHHTT
2nd(s): SSSSSSSSSSSSSSOOOOOOOOSSSSSSSSSSSSOHHHOOOOHHHHHHHHHHHHHHHOOO
Switch: 00000000000000000000000000000000000000000000000000000000110

[120]
1st   : AEEIYLEVRVSNYPAIALYEKLNFKKVKVLKGYYADGEDAYLMARPL
2nd(r):  SEEEEEEETT HHHHHHHHHTT EEEEEETT STTS  EEEEEEE
2nd(s): OOSSSSSSSOOOHHHHHHHHHOOOSSSSSSOOOOOOOOOSSSSSSSO
Switch: 000000000000000000000000000000000000000000000001?


>4R9MA

[0]
1st   : MPSAHSVKLRPLEREDLRYVHQLDNNASVMRYWFEEPYEAFVELSDLYDKHIHDQSERRF
2nd(r):       EEEEE  GGGHHHHHTT ***   EEETTEEE SHHHHHHHHHHTTT TT EEE
2nd(s): OOOOOOSSSSSOOHHHHHHHHHOOODDDOOOSSSOOSSSOOHHHHHHHHHHOOOOOOOSSS
Switch: ????000000000110000001111???111111001110000000000001000000000

[60]
1st   : VVECDGEKAGLVELVEINHVHRRAEFQIIISPEYQGKGLATRAAKLAMDYGFTVLNLYKL
2nd(r): EEEETTEEEEEEEEEEEETTTTEEEEEEEE GGGTTSSHHHHHHHHHHHHHHTS  SEE
2nd(s): SSSSOOSSSSSSSSSSSSOOOOSSSSSSSSOHHHOOOOHHHHHHHHHHHHHHHOOOOOSS
Switch: 000000111000000000000000000000000000000000000000000001000000

[120]
1st   : YLIVDKENEKAIHIYRKLGFSVEGELMHEFFINGQYRNAIRMCIFQHQYLAEHKTPGQTL
2nd(r): EEEEETT HHHHHHHHHTT EEEEEEEEEEE SSSEEEEEEEEEEHHHHHH ********
2nd(s): SSSSSOOOHHHHHHHHHOOOSSSSSSSSSSSOOOOSSSSSSSSSSHHHHHHODDDDDDDDD
Switch: 000000000000000001000000000000010010000000000000011??000000

[180]
1st   : LKPTAQ
2nd(r): ******
2nd(s): DDDDDD
Switch: 000000
```

```
>4RI1A

[0]
1st   : MKKNYSYKNIQAIDFTNLNDGEKLLVLEFRNHPNTALWMYSTFISLKTHLQFIEDLKNSP
2nd(r): *   EEETTEEEEEGGG  HHHHHHHHHHHHSHHHHTTSSSS   HHHHHHHHHHHTT T
2nd(s): DOOOSSSOOSSSSSHHHOOHHHHHHHHHHHHOHHHHOOOOOOOOOOHHHHHHHHHHHHOOOO
Switch: 00000000000000000000000000000000000000000000000000000001100

[60]
1st   : NHRYFLFKEEGVYLGVGSITKINFFHKHGYLGIYKNPFLKNGGETILKALEFIAFEEFQL
2nd(r): T EEEEEEETTEEEEEEEEEEETTTTEEEEEEEE TTSS  HHHHHHHHHHIIIIIS
2nd(s): OOSSSSSSSOOSSSSSSSSSSSOOOOSSSSSSSOOOOOOOHHHHHHHHHHHHHHHOOO
Switch: 00000000000000000000000000000000000000000000000000000000000

[120]
1st   : HSLHLEVMENNFKAIAFYEKNHYELEGRLKGFISKDKEFIDVLLYYKDKKGYNDQSLLKL
2nd(r): SEEEEEEETT HHHHHHHHHTT EEEEEEEEEEEETTEEEEEEEEEEHHHHHHHHH  *
2nd(s): OSSSSSSSOOOHHHHHHHHHOOOSSSSSSSSSSSSOOSSSSSSSSSSHHHHHHHHHOOD
Switch: 00000000000000000000000000000000000000000000000000111?1??


>4U9VB

[0]
1st   : MGRKSSKAKEKKQKRLEERAAMDAVCAKVDAANRLGDPLEAFPVFKKYDRNGLNVSIECK
2nd(r): ********************** HHHHHHHHHT S GGGG GGGGEE  TT  EEEEEE
2nd(s): DDDDDDDDDDDDDDDDDDDDDDOHHHHHHHHHOOOOHHHHOHHHHSSOOOOOOSSSSSS
Switch: 0000000000000??????????10000000001000111100000001100110000000

[60]
1st   : RVSGLEPATVDWAFDLTKTNMQTMYEQSEWGWKDREKREEMTDDRAWYLIAWENSSVPVA
2nd(r): EGGGS HHHHHHHHHHHHHHHHHHHHTSSS   HHHHHHHHH TT EEEEEEETTTEEEE
2nd(s): SHHHOOHHHHHHHHHHHHHHHHHHHHOOOOOOOHHHHHHHHHOOOOSSSSSSSOOOSSSS
Switch: 00000000000000000000000000000000000000001000000000011001000

[120]
1st   : FSHFRFDVECGDEVLYCYEVQLESKVRRKGLGKFLIQILQLMANSTQMKKVMLTVFKHNH
2nd(r): EEEEEEEEETTEEEEEEEEEE GGG SSSHHHHHHHHHHHHHHHTT SEEEEEEETT H
2nd(s): SSSSSSSSSOOSSSSSSSSSSOHHHOOOOHHHHHHHHHHHHHHHOOOOSSSSSSSOOOH
Switch: 00000000000000000000000000000000000000000000100000000000000
```

```
[180]
1st   : GAYQFFREALQFEIDDSSPSMSGCCGEDCSYEILSRRTKFGDSHHSHAGGHCGGCCH
2nd(r): HHHHIIIIIS  EE TTS  TTTBTTB  SEEEEEEE  *****************
2nd(s): HHHHHHHHHOOOSSOOOOOOOOOSOOSOOOSSSSSSSOOODDDDDDDDDDDDDDDD
Switch: 00000000000000000000???????0000000000000000000000000000
```

>4UA3A

```
[0]
1st   : MHFLKQYLFYSPRRMKTQEIKNVTLEDVDFLKNLGVWVEIYHHLEKGLLQQCFNLVKKNM
2nd(r): ***********    *******   S HHHHHTTTEEEEEESS  HHHHHHHHHHHHHHH
2nd(s): DDDDDDDDDDDOOOODDDDDDDOOOOOHHHHHOOOSSSSSSOOOOHHHHHHHHHHHHHH
Switch: 000000000000111??????0000000000000000000000000000000000000

[60]
1st   : EALYRQSSFGWDDSEKLKEMEMEKLEYICIFEKTSKKLVGFLSFEDTVEAGLTCLYIYEI
2nd(r): HHHHHHSTT   HHHHHHHHT TT EEEEEEETTT  EEEEEEEEEEETTEEEEEEEE
2nd(s): HHHHHHOOOOOOHHHHHHHHOOOOOSSSSSSSOOOOOSSSSSSSSSSSOOSSSSSSSS
Switch: 000000000000000000000000000000000000000000000000000000000

[120]
1st   : QLDEHIRGRNVGKWLLKNASILAYRRNLKYIFLTVFSANLNALNFYHHFDFVPHESSPQE
2nd(r): EE GGGTTSSHHHHHHHHHHHHHHTT  EEEEEEETT HHHHHHHHHTT EE TTS
2nd(s): SSOHHHOOOOHHHHHHHHHHHHHHHOOOOSSSSSSSOOOHHHHHHHHHOOOSSOOOOOOO
Switch: 000000000000000000000000000000000000000000000000000000000

[180]
1st   : KKFRSGKVIHPDYYILYTKSRKDW
2nd(r): EE TTS EE  SEEEEEEE  S
2nd(s): SSOOOOOSSOOOSSSSSSSOOOOO
Switch: 00000000000000000000000
```

>5GI5A

```
[0]
1st   : MEVQKLPDQSLISSMMLDSRCGLNDLYPIARLTQKMEDALTVSGKPAACPVDQDCPYTIE
2nd(r): ********************************************** GGG  EEEE
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDOHHHOOSSSS
Switch: 000000000000000000000000000000000000000000000000???1?01000
```

```
[60]
1st   : LIQPEDGEAVIAMLKTFFFKDEPLNTFLDLGECKELEKYSLKPLPDNCSYKAVNKKGEII
2nd(r): E  GGGHHHHHHHHHHTHHHHSHHHHHHT  S HHHHHHHHTTGGGS  EEEEETTS EE
2nd(s): SOOHHHHHHHHHHHHHOHHHHOHHHHHHOOOOOHHHHHHHHOOHHHOOOSSSSSOOOOSS
Switch: 00000000000000001100000000000000000000000000000000001000000

[120]
1st   : GVFLNGLMRRPSPDDVPEKAADSCEHPKFKKILSLMDHVEEQFNIFDVYPDEELILDGKI
2nd(r): EEEEEEEEE     ****** TT   HHHHHHHHHHHHHHHH  HHHHSTT SEEEEEEE
2nd(s): SSSSSSSSSOOOOODDDDDDOOOOOOHHHHHHHHHHHHHHHHHOOHHHHOOOOOSSSSSSS
Switch: 000000000000??????11100000000000000000000000000000000000000

[180]
1st   : LSVDTNYRGLGIAGRLTERAYEYMRENGINVYHVLCSSHYSARVMEKLGFHEVFRMQFAD
2nd(r): EEE GGGTTSSHHHHHHHHHHHHHHHT  EEEEEESSHHHHHHHHHTT EEEEEEEGGG
2nd(s): SSSOHHHOOOOHHHHHHHHHHHHHHHHOOOSSSSSSOOHHHHHHHHHHOOOSSSSSSSHHH
Switch: 00000000000000000000000001000000000000000000000000001000

[240]
1st   : YKPQGEVVFKPAAPHVGIQVMAKEVGPAKAAQTKL
2nd(r):   GGGS      TT  EEEEEEEE **********
2nd(s): OOHHHOOOOOOOOOOSSSSSSSSODDDDDDDDDD
Switch: 00111000000011101000000000000000


>5HGZA

[0]
1st   : MTEVVPSSALSEVSLRLLCHDDIDTVKHLCGDWFPIEYPDSWYRDITSNKKFFSLAATYR
2nd(r):   HHHHHHHTTSEEEEE  GGGHHHHHHHHHHH SS   HHHHHHHHH TTEEEEEEEET
2nd(s): OOHHHHHHHOOOSSSSSOOHHHHHHHHHHHHHHOOOOOOHHHHHHHHHOOOSSSSSSSSO
Switch: ??1111110111000000000000000000000000000000011000100000000

[60]
1st   : GAIVGMIVAEIKNRTKIHKEDGDILASNFSVDTQVAYILSLGVVKEFRKHGIGSLLLESL
2nd(r): TEEEEEEEEEEEEGGGS GGGTTSS TTS TT EEEEEEEEE GGGTTSSHHHHHHHHH
2nd(s): OSSSSSSSSSSSSHHHOOHHHOOOOOOOOOOOOSSSSSSSSSSOHHHOOOOHHHHHHHHH
Switch: 000000000000000000000001110????000000000000000000000000000
```

```
[120]
1st   : KDHISTTAQDHCKAIYLHVLTTNNTAINFYENRDFKQHHYLPYYYSIRGVLKDGFTYVLY
2nd(r): HHHHHHHHTTTEEEEEEEEETT HHHHHHHHTTT EEEEEEEEEEEETTEEEEEEEEEEE
2nd(s): HHHHHHHHOOOSSSSSSSSSOOOHHHHHHHHOOOOSSSSSSSSSSSOOSSSSSSSSSS
Switch: 00000011111110000000000000000001000000000110001010011000000

[180]
1st   : INGGHPPWTILDYIQHLGSALASLSPCSIPHRVYRQAHSLLCSFLPWSGISSKSGIEYSR
2nd(r):  TT      HHHHHHHHHHHHTTS GGGS  ****************************
2nd(s): OOOOOOOOOHHHHHHHHHHHHOOOOHHHOOODDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 00?????????????????1???????????000000000000000000000000000

[240]
1st   : TM
2nd(r): **
2nd(s): DD
Switch: 00


>5JPHA

[-1]
1st   : AMFSKVNNQKMLEDCFYIRKKVFVEEQGVPEESEIDEYESESIHLIGYDNGQPVATARIR
2nd(r):   EEE  SHHHHHHHHHHHIIIIIIIT   HHHHS TTTTTSEEEEEEETTEEEEEEEEE
2nd(s): OOSSSOOOHHHHHHHHHHHHHHHHHHHOOOOHHHHOOOOOOOOSSSSSSSOOSSSSSSSS
Switch: 01000000000000000000000000000000010000000000000000000000000

[59]
1st   : PINETTVKIERVAVMKSHRGQGMGRMLMQAVESLAKDEGFYVATMNAQCHAIPFYESLNF
2nd(r): E SSSEEEEEEEEE GGGTTSSHHHHHHHHHHHHHHTT  EEEEEEEGGGHHHHHHTT
2nd(s): SOOOOSSSSSSSSSOHHHOOOOHHHHHHHHHHHHHHHOOOOSSSSSSSHHHHHHHHHOOO
Switch: 00000000000000000000110000000000000000000000000111110000000000

[119]
1st   : KMRGNIFLEEGIEHIEMTKKLTSLN
2nd(r): EEEEEEEEETTEEEEEEEEE  ***
2nd(s): SSSSSSSSSOOSSSSSSSSSOODDD
Switch: 000111111001111000000??0
```

```
>5K04A

[0]
1st   : MATERDQEIIDFIDQGNYTYAQSLITKKLAKSPQKLFYHVLQNEIHLKSGQRELAIKKNL
2nd(r): ******* HHHHHHHH * HHHHHHHHHHHH  ** HHHHHHHHHHHHHH SHHHHHHHH
2nd(s): DDDDDDDOHHHHHHHHHODOHHHHHHHHHHHHHOODDOHHHHHHHHHHHHHHHOOHHHHHHHH
Switch: 0000000??????????1??????????????00?10000000000001??10000000

[60]
1st   : ELLNRYPNDPLTIEKLSDFFSKMEMEKESSLVYENAIKKYPVSTETLCLSWFDNSIEKYD
2nd(r): HHHHT    HHHHHHHHHHHHHTT HHHHHHHHHHHHHH GGGHHHHHHHHHHHHTTS
2nd(s): HHHHOOOOOHHHHHHHHHHHHHOOOHHHHHHHHHHHHHHHOHHHHHHHHHHHHHHHOOOOO
Switch: 00001?000100000000000100110000000000000000000000000011100

[120]
1st   : FKVFNRIFMYLNKNGKSRLHTLWYAFSFHLLLQEGETDKASLYNSLGKKLMEGLQPFENT
2nd(r): HHHHHHHHHHHHHT   HHHHHHHHHHHHHHHTT  HHHHHHHHHHHHHHHTT S  SH
2nd(s): HHHHHHHHHHHHHOOOOHHHHHHHHHHHHHHHOOOOHHHHHHHHHHHHHHHHOOOOOOOH
Switch: 1110000000001??000000000000000000?000000000000000000000000

[180]
1st   : QEIYVYTLFLSSKEIEQVLSGVTLPLDLELKLLYMKAMKENASFEALHAYTEKLLFKEKF
2nd(r): HHHHHHHTT  HHHHHHHHTT  S   HHHHHHHHHHHHHTT HHHHHHHHHHHHHS
2nd(s): HHHHHHHOOOOHHHHHHHHOOOOOOOOHHHHHHHHHHHHHOOOHHHHHHHHHHHHHOOO
Switch: 000000000000000000010000000000000000000000000000000000000000

[240]
1st   : DDFDTWKLWILSGKEIGKSFEELDQKLTSPTRNISLLKIELDILYSRNIETSVENYYQKF
2nd(r):   HHHHHHHHHHHHTT  HHHHHTT  S  HHHHHHHHHHHHTT  SHHHHHHHHHH
2nd(s): OOHHHHHHHHHHHHHOOOOHHHHHOOOOOOOHHHHHHHHHHHHHOOOOOHHHHHHHHHH
Switch: 000000000000000000000001000000000000000000000000000000000000

[300]
1st   : NTKLCCYADLSQYELPTSFIGSLKNSTSEENLITVVNNRKFVNQTDNWDVYERFSTKEGA
2nd(r): TTSTTHHHHHTTS   HHHHH    ***  SHHHHHHHHHHTT    HHHHHHS S  SS
2nd(s): OOOOOHHHHHOOOOOOHHHHHOOOODDDOOOHHHHHHHHHHOOOOOOHHHHHHOOOOOOO
Switch: 000010000000000000001?????000000000000000010000000000001000000
```

```
[360]
1st   : EYDSNPVNELTLRTIVSDLDSSPQNTIKNIVLLKHLLEQDKYNYKLKLWLMKLYSQLNTN
2nd(r): TTS  THHHHHHHHHHHH  S HHHHHHHHHHHHHHHHHSTT HHHHHHHHHHHTTBS G
2nd(s): OOOOOOHHHHHHHHHHHHOOOOHHHHHHHHHHHHHHHHHOOOOHHHHHHHHHHHOOSOOH
Switch: 00000000000000000000000000000000000000000000000000000000000

[420]
1st   : DLIFPIYNGLKIRMTQHETLNYYLTTTNPSKINLDAWVDIYRFYLTSKQEIKESIIQGFD
2nd(r): GGSHHHHHHTT  THHHHHHGGGGTT    HHHHHHHHHHHHHHHHHHHHHHHHHHHHH
2nd(s): HHOHHHHHHOOOOOHHHHHHHHHHOOOOOOHHHHHHHHHHHHHHHHHHHHHHHHHHHH
Switch: 00100000000000000000000000000000000000000000000000000000000

[480]
1st   : NGVFNKLEGFINFSKRMQNSISLNFTVAKILQISTILGTDGYLNYFIHYLKTNEALIVSD
2nd(r): TT HHHHHHHHHHHHHHHTBHHHHHHHHHHHHHHHHTT HHHHHHHHHHHH HHHHTS
2nd(s): OOOHHHHHHHHHHHHHHHOSHHHHHHHHHHHHHHHHOOOHHHHHHHHHHHHHOHHHOOO
Switch: 00000000000000000000000000000000000001110000000000000000000

[540]
1st   : YTDNRDFKSEWNGLEKIDCIDVPVNDVATKLKLLVYSIVFEDQDASRLLKVFNKITSNAK
2nd(r):  B    SSGGGTTS   S       HHHHHHHHHHHHHHT SS  HHHHHHHHHHTT
2nd(s): OSOOOOOOHHHOOOOOOOOOOOOOOHHHHHHHHHHHHHHHOOOOOOHHHHHHHHHHHOOOO
Switch: 00000000000000000000000000000000000000000000000000000001000

[600]
1st   : FSVFDNLLYKLYFNLLKITKTKLNPQETQSLYNYLQKNLKTDKLKILIPENLLSGELTQN
2nd(r):   HHHHHHHHHHHHHHHHHHS   HHHHHHHHHHHHHHSSHHHHGGGS SSTTBTHHHHH
2nd(s): OOHHHHHHHHHHHHHHHHHHHOOOOHHHHHHHHHHHHHHHOOHHHHHHHOOOOOOSOHHHHH
Switch: 00000000000000000000??000000000000000000000000000000000000

[660]
1st   : LTNLVEFIKIVKLLAKRHPSSYMNQLVNLVKPFGKEFKNLKLVQRQHEIIDSMDFEPPIS
2nd(r): HHHHHHHHHHHHHHHHHS  HHHHHHHHHHTTHHHHHHTT HHHHHHHHHHH     SS
2nd(s): HHHHHHHHHHHHHHHHHHOOOHHHHHHHHHHHOOHHHHHHOOOHHHHHHHHHHHHOOOOOOOO
Switch: 00000000000000000000000000000100000000000000000000000100000000

[720]
1st   : VDISQTKLEIKSSIEDCVVALLNSL
2nd(r):   SHHHHHHHHHHHHHHHHHHHTT
2nd(s): OOOHHHHHHHHHHHHHHHHHHHOOO
Switch: 00100000000000000000000110
```

```
>5K9NA

[0]
1st   : MAKPIADDIVVRQVDVGETEQLMTFLLAHYYPEEPLTAGTHPPEPEAADKEFLLSNVPFG
2nd(r): ******   EEEE  TTS HHHHHHHHHHTTTT HHHHTSSS S  HHHHHHHHTTGGGT
2nd(s): DDDDDDOOOSSSSOOOOOOHHHHHHHHHHOOOOOHHHHOOOOOOOOHHHHHHHHHOOHHHO
Switch: 000000?00000000111100000000000000000010000000000000000000000

[60]
1st   : TCFVALHEGRIVAAVVAGPKDSHEPEHMAEEARKYAGGKWGSILHLLSAVETATDVCRRF
2nd(r):   EEEEETTEEEEEEEEEEE TTHHHHHHHHHHHHTTSHHHHHHHHHHHHHHHHH HHHHT
2nd(s): OOSSSSSOOSSSSSSSSSSSOOOHHHHHHHHHHHHHHOOOHHHHHHHHHHHHHHHHHOHHHHO
Switch: 000000000000000000000000000000000000000000000000000000000000000

[120]
1st   : SVPSCLHVHALGVDPQLRGRNLGGRLMETVAQRGRDLGHQLVSVDCTSVYSARLVQRLGY
2nd(r): T S EEEEEEEEE GGGTTS HHHHHHHHHHHHHHHHT  EEEEEE SHHHHHHHHHTT
2nd(s): OOOOSSSSSSSSSOHHHOOOOHHHHHHHHHHHHHHHHHOOOSSSSSSOOHHHHHHHHHHOOO
Switch: 000000000000000000000000000000000010000000000000000000000000

[180]
1st   : QLINTLRYVDHLDASGQQVIRPPPPHESVQTFVLHL
2nd(r): EEEEEEEGGG B TTS BS    TT  EEEEEEEE
2nd(s): SSSSSSSHHHOSOOOOOSOOOOOOOOOSSSSSSSSO
Switch: 000000000000000000000000000000000000


>5KTAA

[0]
1st   : MVNFNLKANTTYLRLVEENDAEFICTLRNNDKLNTYISKSTGDIKSQAEWIRNYKNRENN
2nd(r): *    EE SSEEEEE  GGGHHHHHHHHHHHH STT  S    HHHHHHHHHHHHHHHHT
2nd(s): DOOOOSSOOOSSSSSOOHHHHHHHHHHHHHHHHOOOOOOOOOOOHHHHHHHHHHHHHHHHO
Switch: 000001000000000000000000000011110000000000000000000000000000

[60]
1st   : GEEYYFIIFRSDDQSPIGTVRLYDFHENPKSFCWGSWILNEHKTKYAAVESALLVYEAGF
2nd(r): TS EEEEEEETTT  EEEEEEEEEEETTTTEEEEEEEEE TT  TTHHHHHHHHHHIIII
2nd(s): OOOSSSSSSSOOOOOSSSSSSSSSSSOOOOSSSSSSSSSOOOOOOOHHHHHHHHHHHHHH
Switch: 001000000000001000000000000000000000000000000000000000000000
```

```
[120]
1st   : STLGFEQSHFEVMKGNDKVHSFHLKMGAQKISEDDENIYYIFPKSKYKENKIQYARFLGK
2nd(r): IIS  SEEEEEEETT HHHHHHHHHHT EEEEE SSEEEEEEEHHHHHHHHHHTHHHH *
2nd(s): HHOOOOSSSSSSSOOOHHHHHHHHHHOOSSSSSOOOSSSSSSSHHHHHHHHHHOHHHHOD
Switch: 00000000000000000000000000000000000000000000000001111000000?


>5WIFA

[-3]
1st   : MSTTSSVRLRPLEREDLPFVHQLDNNASIMRYWFEEPYEAFVELCDLYDKHIHDQSERRF
2nd(r): ***** EEEEE  GGGHHHHHHT ***   EEETTEEE SHHHHHHHHHHTTT TT EEE
2nd(s): DDDDDOSSSSSOOHHHHHHHHHHOODDDOOOSSSOOSSSOOHHHHHHHHHHOOOOOOOSSS
Switch: ?????0100000000000000100???00000000000000000000000000000000

[60]
1st   : IIESQGTKIGLVELVEINHIHRRAEFQIIIDPTHQGKGYAGAAAKLAMEYGFSVLNLYKL
2nd(r): EEEETTEEEEEEEEEEETTTTEEEEEEEE GGGTTSSHHHHHHHHHHHHHHTS  SEE
2nd(s): SSSSOOSSSSSSSSSSSOOOOSSSSSSSSOHHHOOOOHHHHHHHHHHHHHHOOOOOSS
Switch: 00000000000000000000000000000000011100000000000000001000000

[120]
1st   : YLIVDKENEKAIHIYSKLGFEIEGELKQEFFINGEYRTVIRMCIFQPQYLAKYKTPSIKN
2nd(r): EEEEETT HHHHHHHHHHT EEEEEEEEEEEETTEEEEEEEEEEEHHHHHHHT ******
2nd(s): SSSSSOOOHHHHHHHHHHOOSSSSSSSSSSSSOOSSSSSSSSSSSHHHHHHHOODDDDDDD
Switch: 00000000000000000100000000000000000000000000000000011?00000

[180]
1st   : A
2nd(r): *
2nd(s): D
Switch: 0


>5YGEA

[0]
1st   : MTERPRDCRPVVRRARTSDVPAIKQLVDTYAGKILLEKNLVTLYEAVQEFWVAEHPDLYG
2nd(r): *****      EEE  GGGHHHHHHHHHHHBTTTB    HHHHHHTGGGEEEEE TTTTT
2nd(s): DDDDDOOOOOOSSSOOHHHHHHHHHHHHHHSOOOSOOOOHHHHHHOHHHSSSSSOOOOOO
Switch: 00000??000100000000000000000000000000000000000000000111100
```

```
[60]
1st   : KVVGCGALHVLWSDLGEIRTVAVDPAMTGHGIGHAIVDRLLQVARDLQLQRVFVLTFETE
2nd(r):  EEEEEEEEEEETTEEEEEEEEE GGGTTSSHHHHHHHHHHHHHHHTT  EEEEEES HH
2nd(s): OSSSSSSSSSSSOOSSSSSSSSSSOHHHOOOOHHHHHHHHHHHHHHHHOOOOSSSSSSOOHH
Switch: 10000000000000000000000000000000000000000000000000000000000000

[120]
1st   : FFARHGFTEIEGTPVTAEVFDEMCRSYDIGVAEFLDLSYVKPNILGNSRMLLVL
2nd(r): HHHTTT EE       HHHHHHHHHH SHHHHTT  HHHHS  SS  EEEEEE
2nd(s): HHHOOOOSSOOOOOOOHHHHHHHHHHOOHHHHOOOOHHHHOOOOOOOSSSSSSO
Switch: 00000000000000000000000000000000000000000000000000000000
```

D.2 Test Set

```
>2B4YA

[0]
1st   : MRPLQIVPSRLISQLYCGLKPPASTRNQICLKMARPSSSMADFRKFFAKAKHIVIISGAG
2nd(r): ********************************** B  HHHHHHHHHH SEEEEEE GG
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDOSOOHHHHHHHHHHOOSSSSSSOHH
Switch: 000000000000000000000000000????????0100000000001100000000011

[60]
1st   : VSAESGVPTFRGAGGYWRKWQAQDLATPLAFAHNPSRVWEFYHYRREVMGSKEPNAGHRA
2nd(r): GGGGGT *******  BTTB HHHHSSHHHHHH HHHHHHHHHHHHHHHHT    HHHHH
2nd(s): HHHHHOODDDDDDDOOSOOSOHHHHOOHHHHHHOHHHHHHHHHHHHHHHOOOOOHHHHH
Switch: 11111?????????11100110001001100000111000000000011110000000000

[120]
1st   : IAECETRLGKQGRRVVVITQNIDELHRKAGTKNLLEIHGSLFKTRCTSCGVVAENYKSPI
2nd(r): HHHHHHHHHTTT EEEEEE  SS HHHHHT  SEEETTEEEEEEEETTT  EEE   SSS
2nd(s): HHHHHHHHHOOOOSSSSSSOOOOOHHHHHOOOOSSSOOSSSSSSSSOOOOOSSSOOOOOO
Switch: 000000111110000000000000110010000000000000000000000000000000

[180]
1st   : CPALSGKGAPEPGTQDASIPVEKLPRCEEAGCGGLLRPHVVWFGENLDPAILEEVDRELA
2nd(r): SGGGTT    STT       GGGS B  STTT  BEEEEE  TT    HHHHHHHHHHHH
2nd(s): OHHHOOOOOOOOOOOOOOOOHHHOOSOOOOOOOOSSSSSSOOOOOOOOHHHHHHHHHHHH
Switch: 000000000000000000001110000011100000000000000100000000010001
```

```
[240]
1st   : HCDLCLVVGTSSVVYPAAMFAPQVAARGVPVAEFNTETTPATNRFRFHFQGPCGTTLPEA
2nd(r): H SEEEEES  S STTGGGHHHHHHHTT  EEEEESS  TTGGGSSEEEES HHHHHHHH
2nd(s): HOOSSSSSOOOOOOOOHHHHHHHHHHOOOOSSSSSOOOOOOHHHOOSSSSOOHHHHHHHH
Switch: 10000000100001101111100001100000010?????111?010010011100000

[300]
1st   : LACHENETVS
2nd(r): T ********
2nd(s): OODDDDDDDD
Switch: 1?00000000


>2HJHA

[0]
1st   : MTIPHMKYAVSKTSENKVSNTVSPTQDKDAIRKQPDDIINNDEPSHKKIKVAQPDSLRET
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 000000000000000000000000000000000000000000000000000000000000

[60]
1st   : NTTDPLGHTKAALGEVASMELKPTNDMDPLAVSAASVVSMSNDVLKPETPKGPIIISKNP
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 00000000000000000000000000000000000?????????????????????000

[120]
1st   : SNGIFYGPSFTKRESLNARMFLKYYGAHKFLDTYLPEDLNSLYIYYLIKLLGFEVKDQAL
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: ????????????????????????????????????????????????????????????

[180]
1st   : IGTINSIVHINSQERVQDLGSAISVTNVEDPLAKKQTVRLIKDLQRAINKVLCTRLRLSN
2nd(r): ****************************   EEEEE   B EE *****        TT
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDOOOSSSSSOOOSOSSODDDDDOOOOOOOOOO
Switch: ????????000000000000000000000?001111111111111?????1100000000
```

```
[240]
1st   : FFTIDHFIQKLHTARKILVLTGAGVSTSLGIPDFRSSEGFYSKIKHLGLDDPQDVFNYNI
2nd(r):   SHHHHHHHHHH SSEEEEE GGGGGGGT   SSSTTSHHHHTGGG  SSGGGGGBHHH
2nd(s): OOOHHHHHHHHHHOOOSSSSSOHHHHHHHOOOOOOOOOOHHHHOHHHOOOOHHHHHSHHH
Switch: 00000000000000000000000000000000000000000000010110000000000000

[300]
1st   : FMHDPSVFYNIANMVLPPEKIYSPLHSFIKMLQMKGKLLRNYTQNIDNLESYAGISTDKL
2nd(r): HHH THHHHHHGGGG    S   HHHHHHHHHHHTT EEEEEE   S HHHHTT  TTTE
2nd(s): HHHOOHHHHHHHHHHOOOOOOOOHHHHHHHHHHHHOOOSSSSSSOOOOOHHHHOOOOOOOS
Switch: 00001000000000100000000000000000000000000000000100010001110

[360]
1st   : VQCHGSFATATCVTCHWNLPGERIFNKIRNLELPLCPYCYKKRREYFPEGYNNKVGVAAS
2nd(r): EETTEEEEEEEETTT  EEEGGGGHHHHHTT   B TTTHHHHHHH  ***********
2nd(s): SSOOSSSSSSSSOOOOOSSSHHHHHHHHHOOOOOSOOOOHHHHHHHOODDDDDDDDDDDD
Switch: 00001111000000000000000000000000000000000000000??????000000

[420]
1st   : QGSMSERPPYILNSYGVLKPDITFFGEALPNKFHKSIREDILECDLLICIGTSLKVAPVS
2nd(r): *****   TTS TTTTBEEEEE  BTSB  HHHHHHHHHHTTT  EEEEES    EETGG
2nd(s): DDDDDOOOOOOOOOOOSSSSSSOOSOOSOOHHHHHHHHHHOOOOOSSSSSOOOOOSSOHH
Switch: 00???10000000000000011000000000000000000111000000000000000000

[480]
1st   : EIVNMVPSHVPQVLINRDPVKHAEFDLSLLGYCDDIAAMVAQKCGWTIPHKKWNDLKNKN
2nd(r): GHHHHS TTS EEEEESS  TTS  SEEEES HHHHHHHHHHHHT    STTHHHHHT
2nd(s): HHHHHOOOOOOSSSSSOOOOOOOOOOSSSSOOHHHHHHHHHHHHHOOOOOOOOHHHHHOOO
Switch: 00000010000000000000000000000000000000000010000000000001000

[540]
1st   : FKCQEKDKGVYVVTSDEHPKTL
2nd(r): EEEEEEETTEEEEEE ******
2nd(s): SSSSSSSOOSSSSSSODDDDDD
Switch: 1000011000000001?000000


>4IG9A

[-1]
1st   : MMADEAALALQPGGSPSAAGADREAASSPAGEPLRKRPRRDGPGLERSPGEPGGAAPERE
2nd(r):  ************************************************************
```

```
2nd(s): ODDDD
```

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[419]
1st   : EQFHRAMKYDKDEVDLLIVIGSSLKVRPVALIPSSIPHEVPQILINREPLPHLHFDVELL
2nd(r): HHHHHHHHHHTTT SEEEEES    STTGGGHHHHS TTS EEEEESS  TTS  SEEEE
2nd(s): HHHHHHHHHHOOOOOSSSSSOOOOOOOOOHHHHHHHOOOOOOSSSSSOOOOOOOOOOSSSS
Switch: 00000000000000000000000000000000010000000000000000000000000

[479]
1st   : GDCDVIINELCHRLGGEYAKLCCNPVKLSEITEKPPRTQKELAYLSELPPTPLHVSEDSS
2nd(r): S HHHHHHHHHHHH HHHHTT ************************************
2nd(s): OOHHHHHHHHHHHHHOHHHHOOODDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 00000000000000011001107??????????000000000000000000000000000

[539]
1st   : SPERTSPPDSSVIVTLLDQAAKSNDDLDVSESKGCMEEKPQEVQTSRNVESIAEQMENPD
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 00000000000000000000000000000000000000000000000000000000000

[599]
1st   : LKNVGSSTGEKNERTSVAGTVRKCWPNRVAKEQISRRLDGNQYLFLPPNRYIFHGAEVYS
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 00000000000000000000000000000000000000000000000000000000000

[659]
1st   : DSEDDVLSSSSCGSNSDSGTCQSPSLEEPMEDESEIEEFYNGLEDEPDVPERAGGAGFGT
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 00000000000000000000000000000000000000000000000000000000000

[719]
1st   : DGDDQEAINEAISVKQEVTDMNYPSNKS
2nd(r): ****************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 00000000000000000000000000000
```

```
>4L3OA

[0]
1st   : MAEPDPSHPLETQAGKVQEAQDSDSDSEGGAAGGEADMDFLRNLFSQTLSLGSQKERLLD
2nd(r): ************************************************     S
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDOOOOOO
Switch: OOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOO??OOOO

[60]
1st   : ELTLEGVARYMQSERCRRVICLVGAGISTSAGIPDFRSPSTGLYDNLEKYHLPYPEAIFE
2nd(r): SSSHHHHHHHHTSSS   EEEEE GGGTGGGT   TT ***** TTGGG SSGGGGGB
2nd(s): OOOHHHHHHHHOOOOOOOSSSSSOHHHOHHHOOOOOOODDDDDOOOOHHHOOOOHHHHHS
Switch: OOOOOOOOOOOOOOOOOOOOOOOOO1111OOOOOOO????????1110000000110

[120]
1st   : ISYFKKHPEPFFALAKELYPGQFKPTICHYFMRLLKDKGLLLRCYTQNIDTLERIAGLEQ
2nd(r): HHHHHH  HHHHHHHHHHSTTSS   HHHHHHHHHHHTT EEEEEE  SS HHHHHT  G
2nd(s): HHHHHHOOHHHHHHHHHHOOOOOOOOHHHHHHHHHHHOOOSSSSSSOOOOOHHHHHOOOH
Switch: OOOOOOOOOOOOOO111OOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOO10000

[180]
1st   : EDLVEAHGTFYTSHCVSASCRHEYPLSWMKEKIFSEVTPKCEDCQSLVKPDIVFFGESLP
2nd(r): GGEEETTEEEEEEES TTT  EE HHHHHHHHHT   B SSS  BEEEEE  BTSB
2nd(s): HHSSSOOSSSSSSSSOOOOOOOSSOHHHHHHHHHOOOOOSOOOOOOSSSSSSOOSOOSOO
Switch: OOOOOOOOOOOOOOOOOOOOOOO1OOOOOOOO11OOOOOOOOOOOOOOOOOOOOO100

[240]
1st   : ARFFSCMQSDFLKVDLLLVMGTSLQVQPFASLISKAPLSTPRLLINKEKAGQSDPFLGMI
2nd(r): HHHHHHHHHHTTS SEEEEES    EETTGGGGGSS TT  EEEEESS    S   GGG
2nd(s): HHHHHHHHHHOOOOOSSSSSOOOOOSSOOHHHHHOOOOOOOSSSSSOOOOOOOOOOHHHO
Switch: OOOOO1111OOOOOOOOOOOOOOO11O1OOOOO1OOOOOOOOOOOOOOOOOOOO11??

[300]
1st   : MGLGGGMDFDSKKAYRDVAWLGECDQGCLALAELLGWKKELEDLVRREHASIDAQSGAGV
2nd(r): SS      SSSTT  SEEEEES HHHHHHHHHHHHT HHHHHHHHHHHHHHHHHH ****
2nd(s): OOOOOOOOOOOOOOOOSSSSSOOHHHHHHHHHHHHHOOHHHHHHHHHHHHHHHHHHODDDD
Switch: ?????OOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOO1100000
```

```
[360]
1st   : PNPSTSASPKKSPPPAKDEARTTEREKPQ
2nd(r): ****************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 00000000000000000000000000000
```

```
>5BTRA

[0]
1st   : MADEAALALQPGGSPSAAGADREAASSPAGEPLRKRPRRDGPGLERSPGEPGGAAPEREV
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 000000000000000000000000000000000000000000000000000000000000

[60]
1st   : PAAARGCPGAAAAALWREAEAEAAAAGGEQEAQATAAAGEGDNGPGLQGPSREPPLADNL
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 000000000000000000000000000000000000000000000000000000000000

[120]
1st   : YDEDDDDEGEEEEEAAAAAIGYRDNLLFGDEIITNGFHSCESDEEDRASHASSSDWTPRP
2nd(r): ************************  S  S  EE   *****************   S
2nd(s): DDDDDDDDDDDDDDDDDDDDDDOOOOOOOOOSSOOODDDDDDDDDDDDDDDDDOOOOOOO
Switch: 00000000000000000000??????????????000000000000000000???????

[180]
1st   : RIGPYTFVQQHLMIGTDPRTILKDLLPETIPPPELDDMTLWQIVINILSEPPKRKKRKDI
2nd(r): EE HHHHHHHHHHHT  HHHHHHHH TT    TT  HHHHHHHHHHHHH        SS
2nd(s): SSOHHHHHHHHHHHOOOHHHHHHHHOOOOOOOOOOOHHHHHHHHHHHHHOOOOOOOOOO
Switch: ??000000000011000000000000000000000000000000100000000000

[240]
1st   : NTIEDAVKLLQECKKIIVLTGAGVSVSCGIPDFRSRDGIYARLAVDFPDLPDPQAMFDIE
2nd(r):  SHHHHHHHHHH SSEEEEE GGGSTTTT   SSSTTTHHHHHHHH TT  SGGGGGBHH
2nd(s): OOHHHHHHHHHHOOOSSSSSOHHHOOOOOOOOOOOOOOHHHHHHHHOOOOOOHHHHHSHH
Switch: 000000000000000000000???1111??????????111100110000011000100
```

```
[300]
1st   : YFRKDPRPFFKFAKEIYPGQFQPSLCHKFIALSDKEGKLLRNYTQNIDTLEQVAGIQRII
2nd(r): HHHH  HHHHHHHTTS TTS    HHHHHHHHHHHTT EEEEEE   S HHHHTT SSEE
2nd(s): HHHHOOHHHHHHHOOOOOOOOOOOOHHHHHHHHHHHOOOSSSSSSOOOOOHHHHOOOOOSS
Switch: 00000000000001110111000000000001?110000000000000000001000000

[360]
1st   : QCHGSFATASCLICKYKVDCEAVRGDIFNQVVPRCPRCPADEPLAIMKPEIVFFGENLPE
2nd(r): ETTEEEEEEEETTT  EEEHHHHHHHHHTT   B SSS TT TT BEEEEE  BTSB  H
2nd(s): SOOSSSSSSSSOOOOOSSSHHHHHHHHHOOOOOSOOOOOOOOOOOSSSSSSOOSOOSOOH
Switch: 00000000000000000001000000000000000?????????0000000001001000

[420]
1st   : QFHRAMKYDKDEVDLLIVIGSSLKVRPVALIPSSIPHEVPQILINREPLPHLHFDVELLG
2nd(r): HHHHHHHHHTTT SEEEEES    STTGGGHHHHS TTS EEEEESS  TT   SEEEES
2nd(s): HHHHHHHHHOOOOOSSSSSOOOOOOOOOHHHHHHHOOOOOOSSSSSOOOOOOOOOOSSSSO
Switch: 00000000000000000000000011000010010000000000000000000000000000

[480]
1st   : DCDVIINELCHRLGGEYAKLCCNPVKLSEITEKPPRTQKELAYLSELPPTPLHVSEDSSS
2nd(r):  HHHHHHHHHHHH HHHHT  S TTSSSSS  ****************************
2nd(s): OHHHHHHHHHHHHOHHHHOOOOOOOOOOOOOODDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 00000000000000100010??????????000000000000000000000000000000

[540]
1st   : PERTSPPDSSVIVTLLDQAAKSNDDLDVSESKGCMEEKPQEVQTSRNVESIAEQMENPDL
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 00000000000000000000000000000000000000000000000000000000000000

[600]
1st   : KNVGSSTGEKNERTSVAGTVRKCWPNRVAKEQISRRLDGNQYLFLPPNRYIFHGAEVYSD
2nd(r): ************************************  EEETTTEEE TT    **
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDOOSSSOOOSSSOOOOOOODD
Switch: 00000000000000000000000000000000000?????10000000007???????

[660]
1st   : SEDDVLSSSSCGSNSDSGTCQSPSLEEPMEDESEIEEFYNGLEDEPDVPERAGGAGFGTD
2nd(r): ************************************************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 00000000000000000000000000000000000000000000000000000000000000
```

```
[720]
1st   : GDDQEAINEAISVKQEVTDMNYPSNKS
2nd(r): ***************************
2nd(s): DDDDDDDDDDDDDDDDDDDDDDDDDDD
Switch: 00000000000000000000000000000
```

APPENDIX E

Descriptor Overlays

E.1 Learning Set

Figure E.12: Decriptors for 1CJW:A

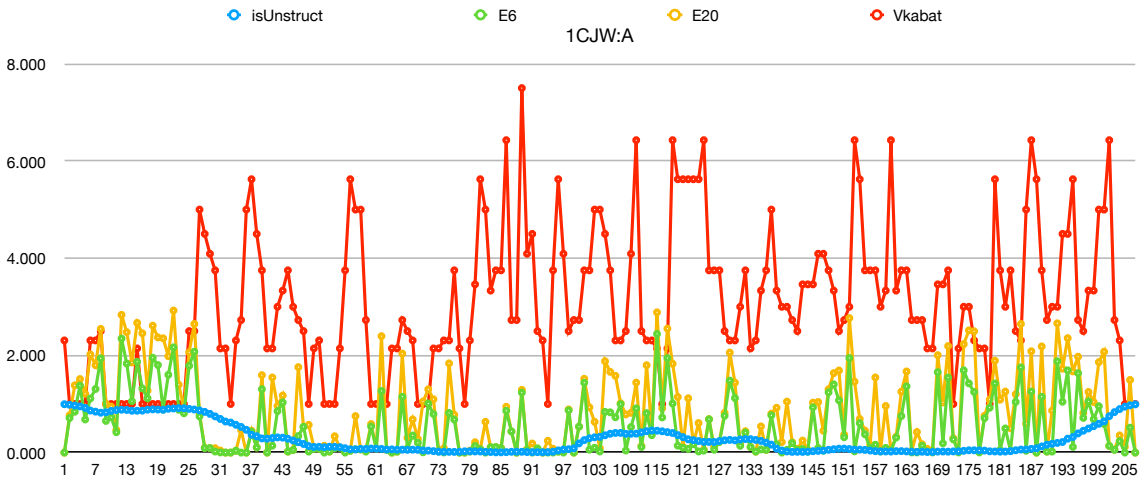


Figure E.13: Decriptors for 1GX3:A

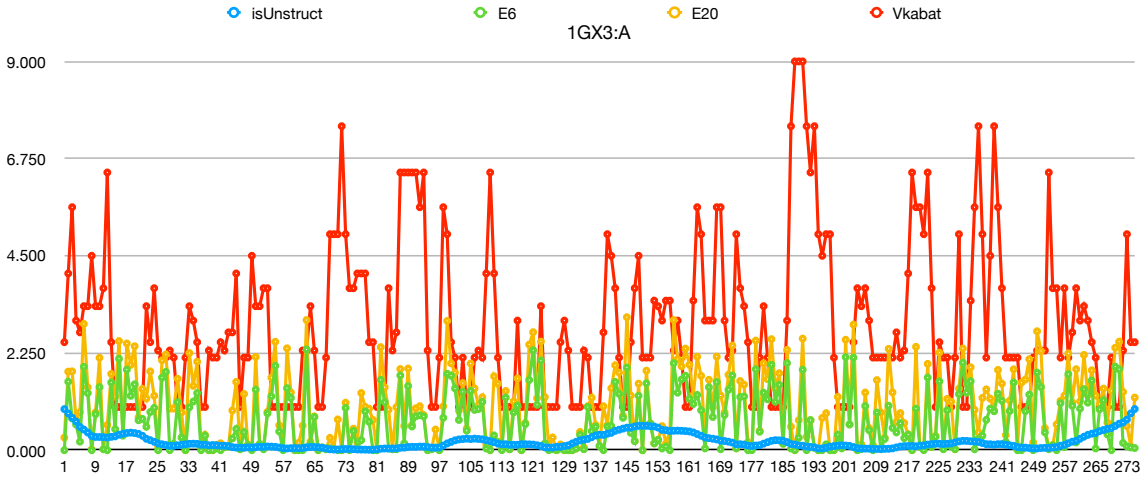


Figure E.14: Decriptors for 1IB1:A

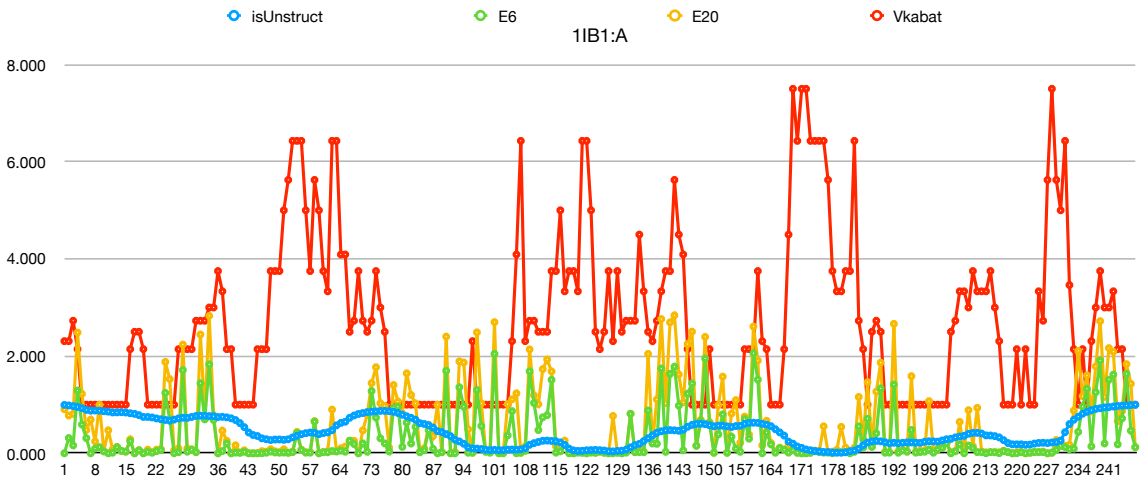


Figure E.15: Decriptors for 1N71:A

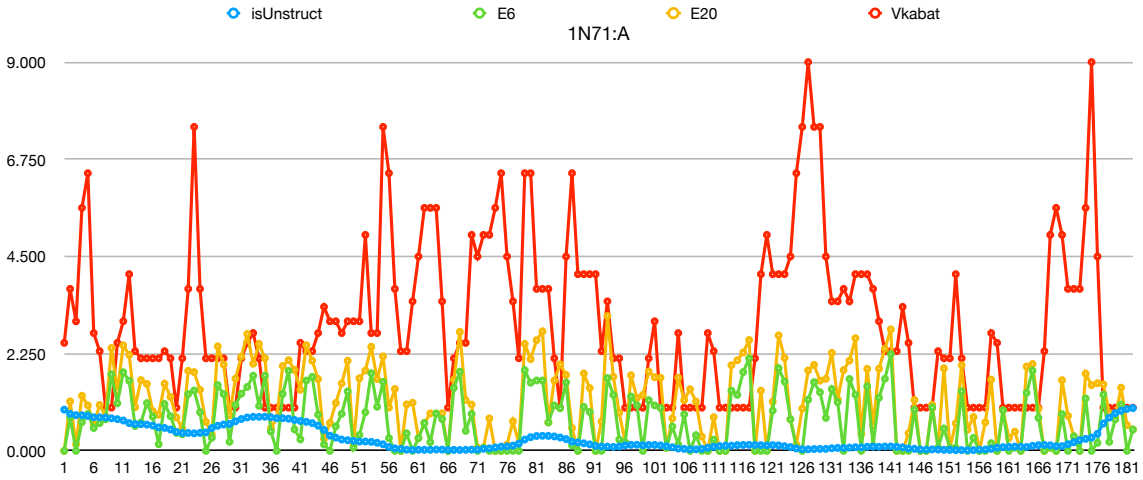


Figure E.16: Decriptors for 1S7F:A

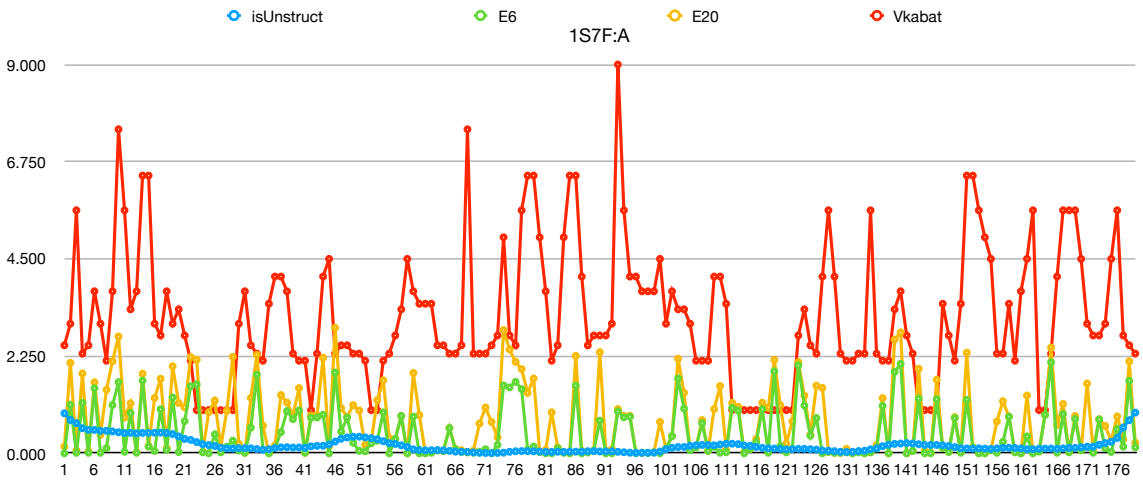


Figure E.17: Decriptors for 1TIQ:A

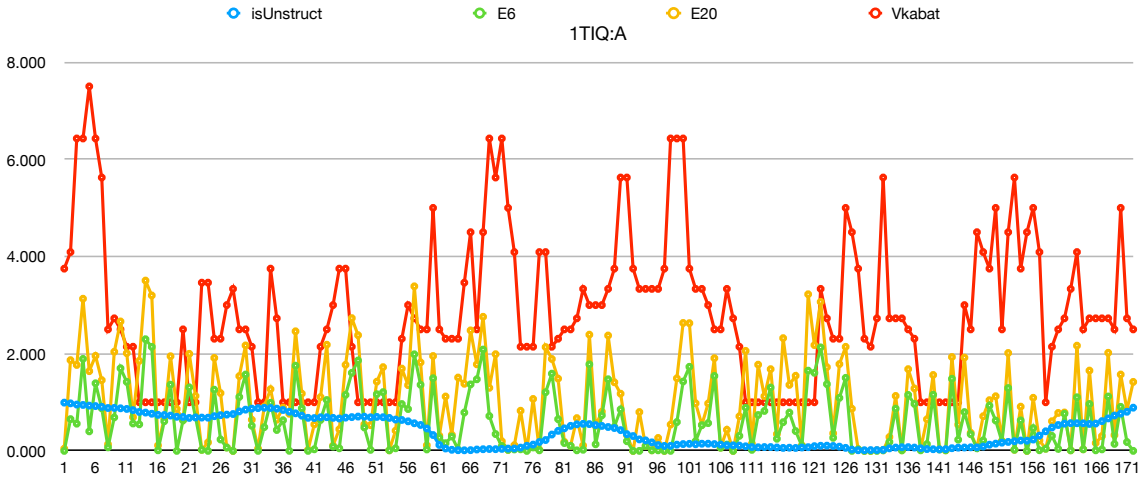


Figure E.18: Decriptors for 1XEB:A

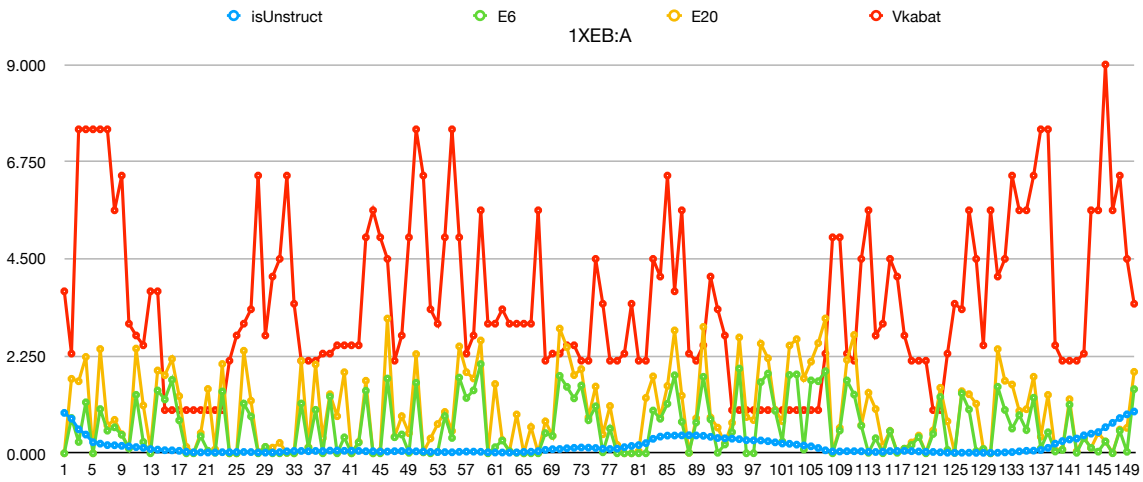


Figure E.19: Decriptors for 2B5G:A

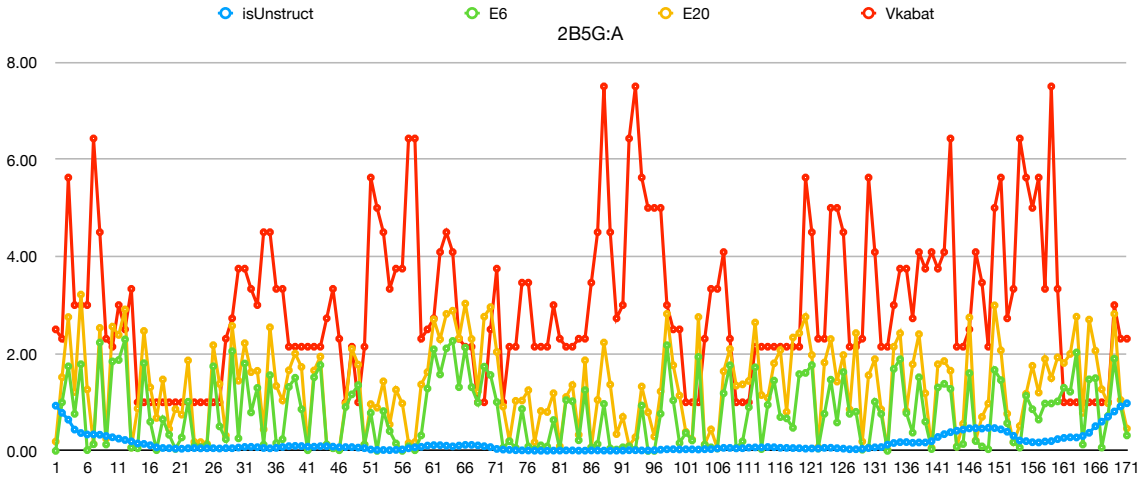


Figure E.20: Decriptors for 2BL1:A

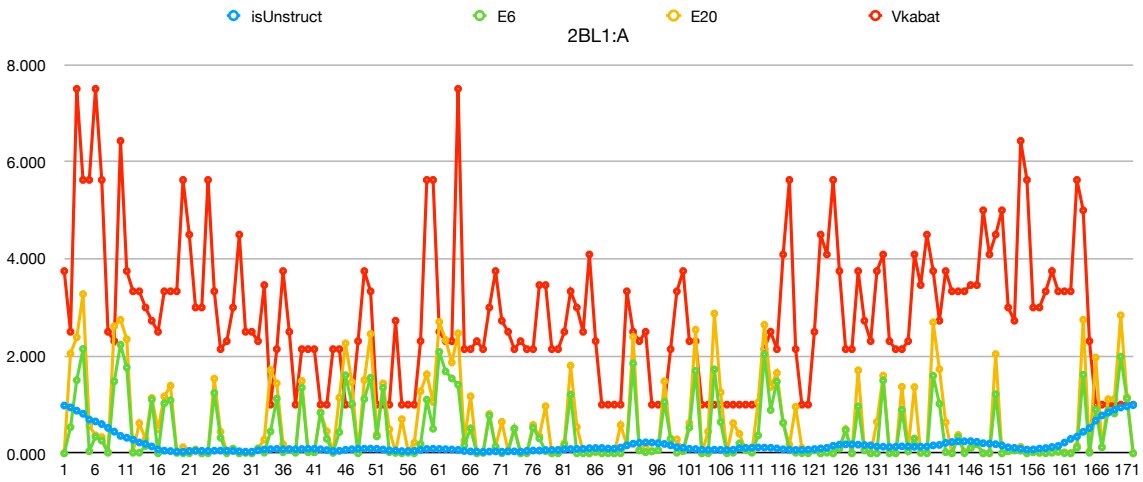


Figure E.21: Decriptors for 2FIA:A

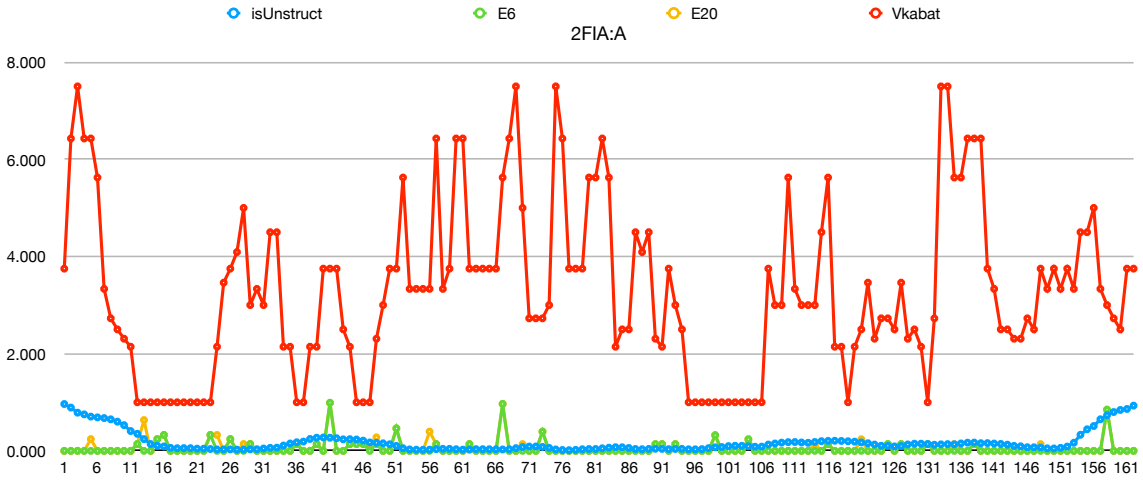


Figure E.22: Decriptors for 2JLM:A

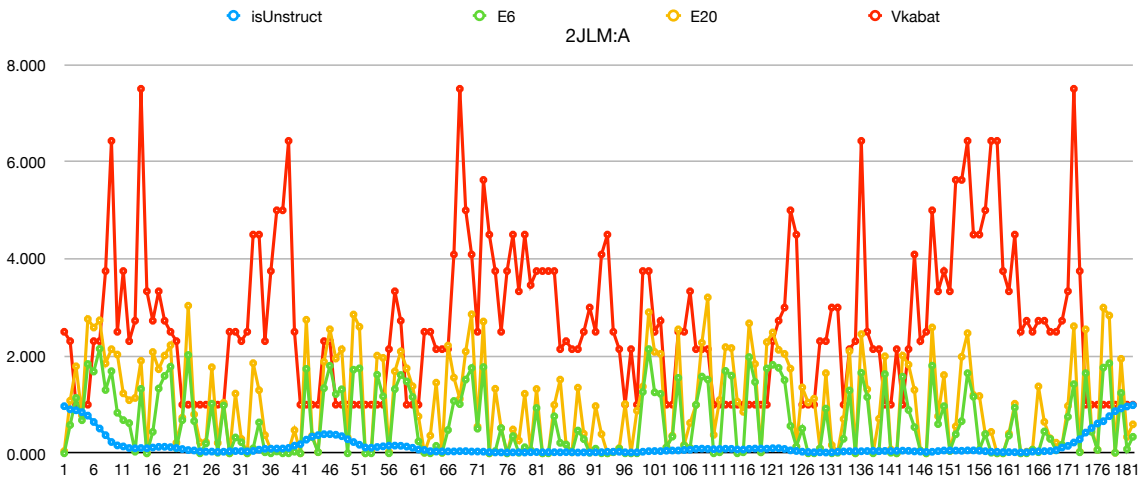


Figure E.23: Decriptors for 2QV4:A

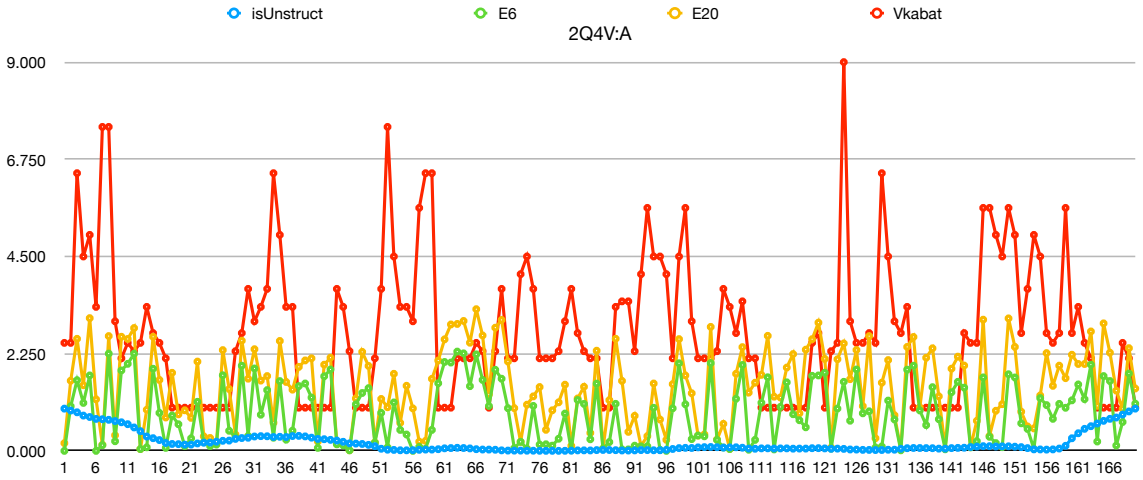


Figure E.24: Decriptors for 2REE:A

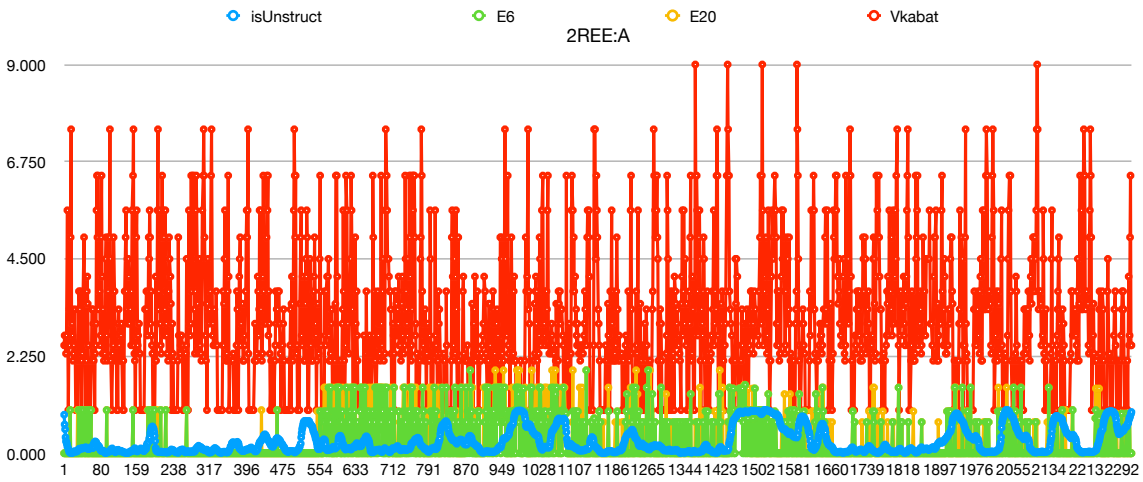


Figure E.25: Decriptors for 2VFB:A

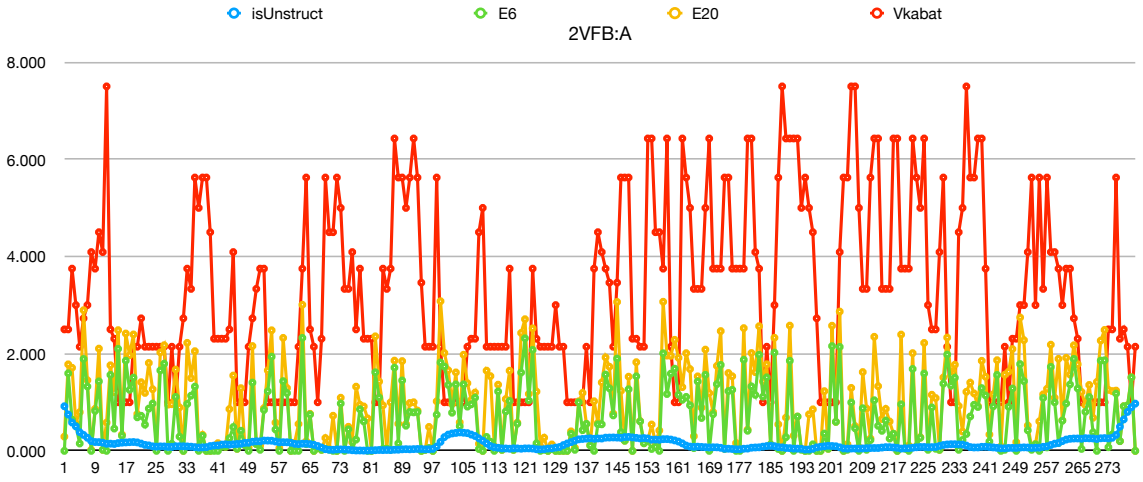


Figure E.26: Decriptors for 2VI7:A

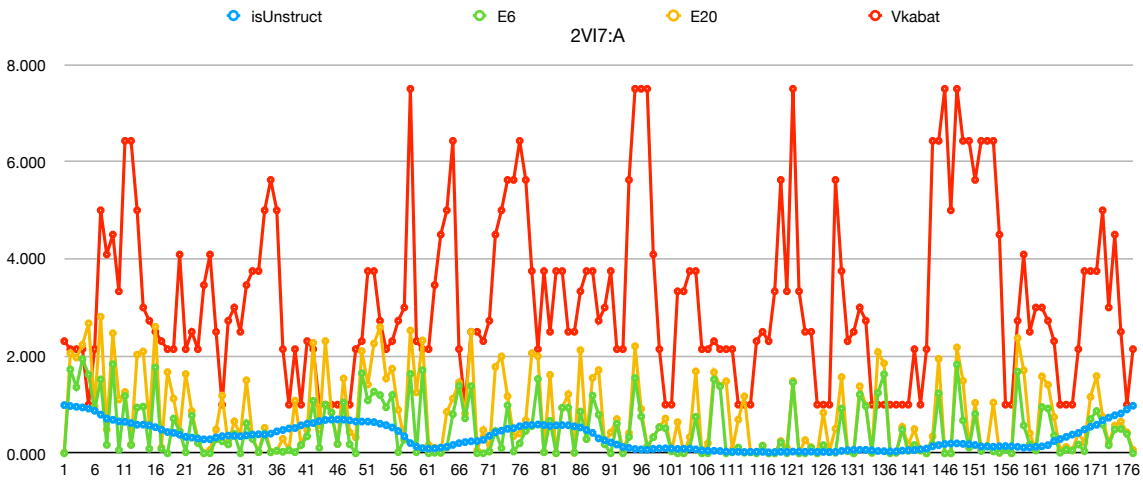


Figure E.27: Decriptors for 2WPW:A

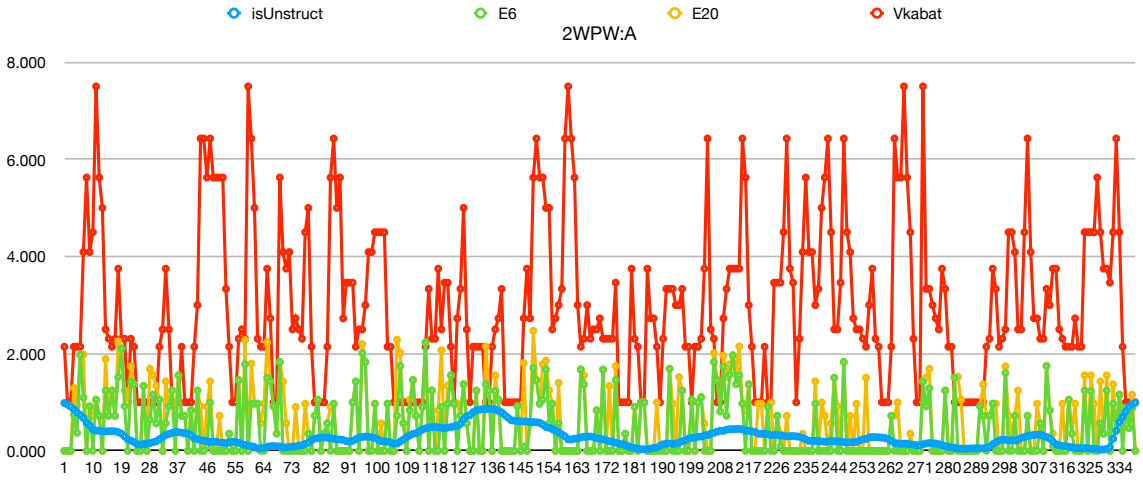


Figure E.28: Decriptors for 3FS8:A

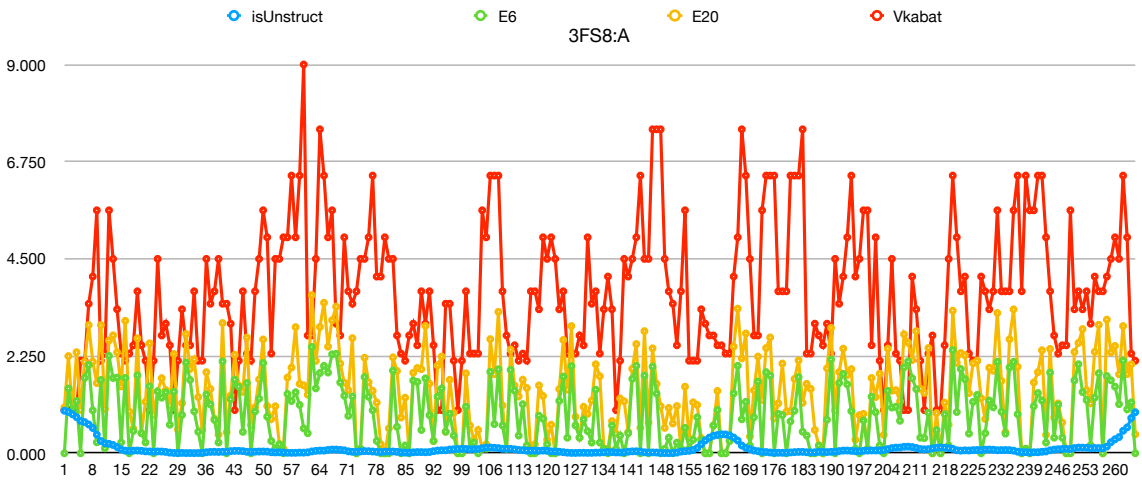


Figure E.29: Decriptors for 3MQH:A

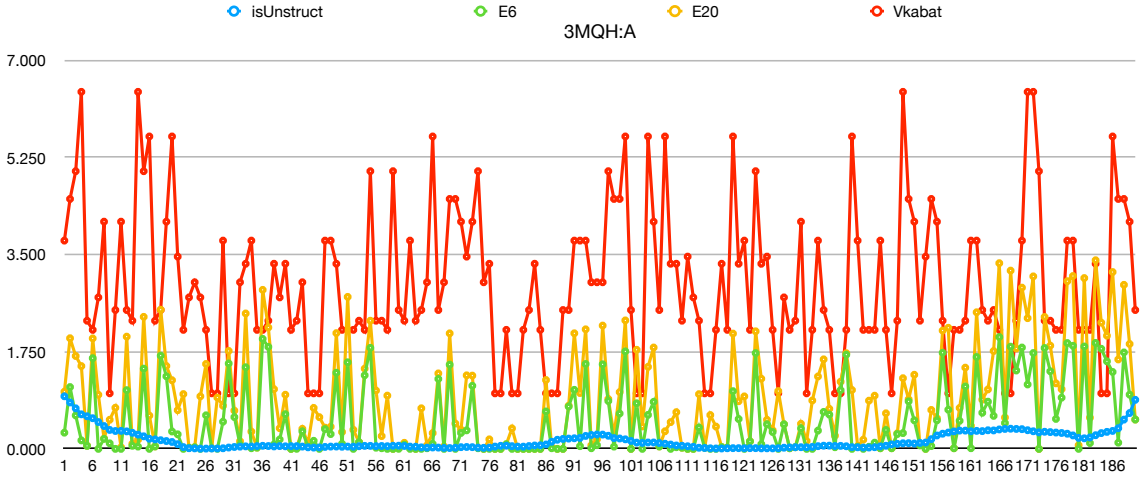


Figure E.30: Decriptors for 3N37:A

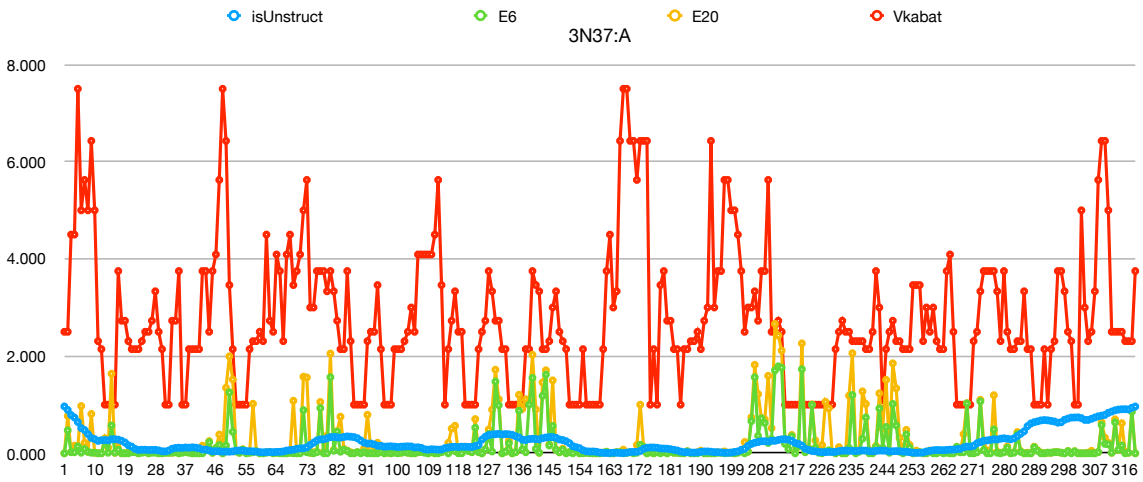


Figure E.31: Decriptors for 3NE7:A

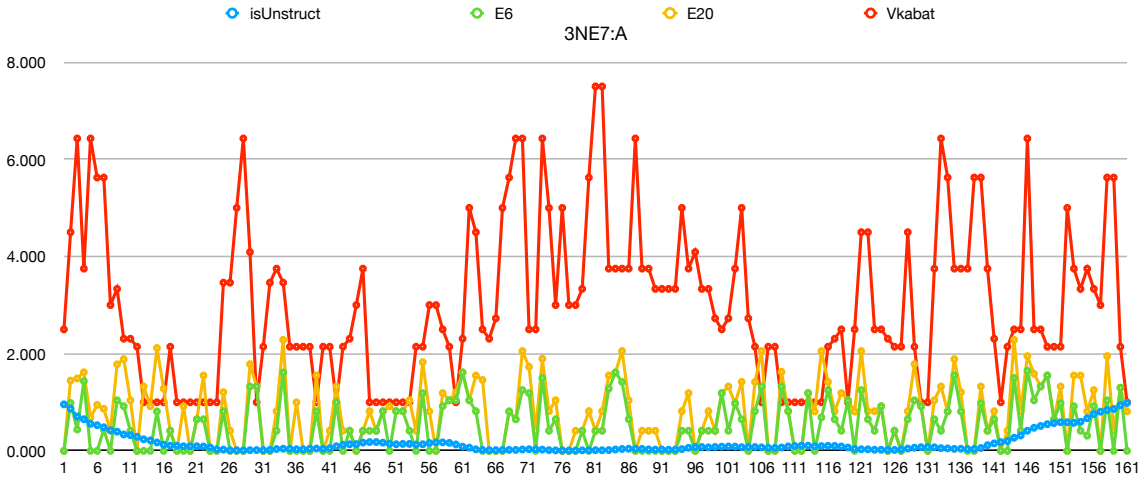


Figure E.32: Decriptors for 3QB8:A

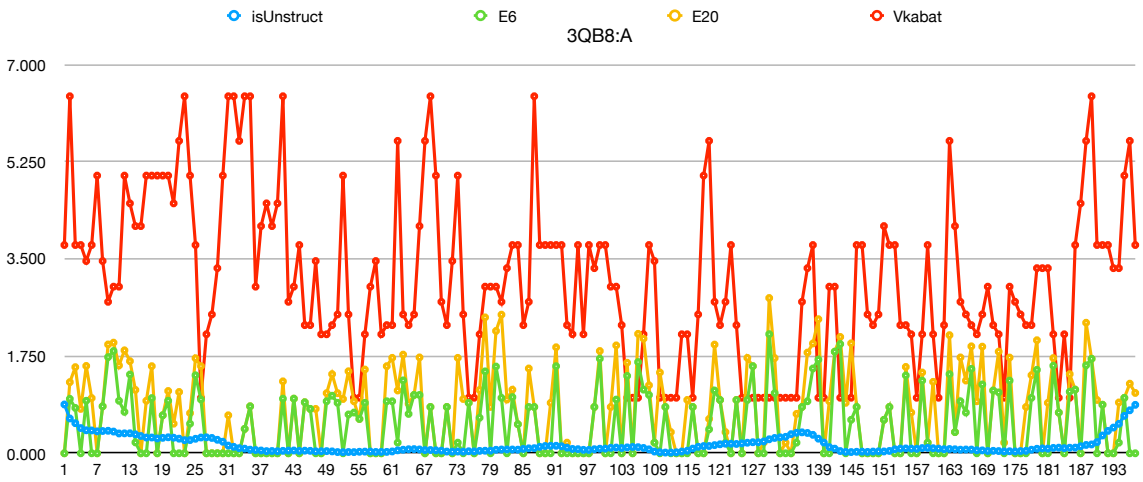


Figure E.33: Decriptors for 3SMA:A

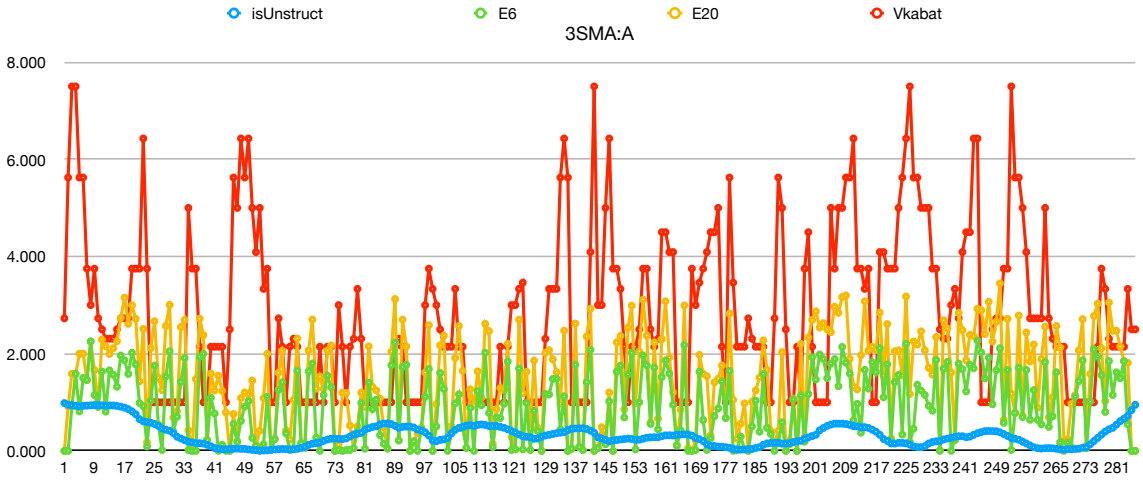


Figure E.34: Decriptors for 3TFY:A

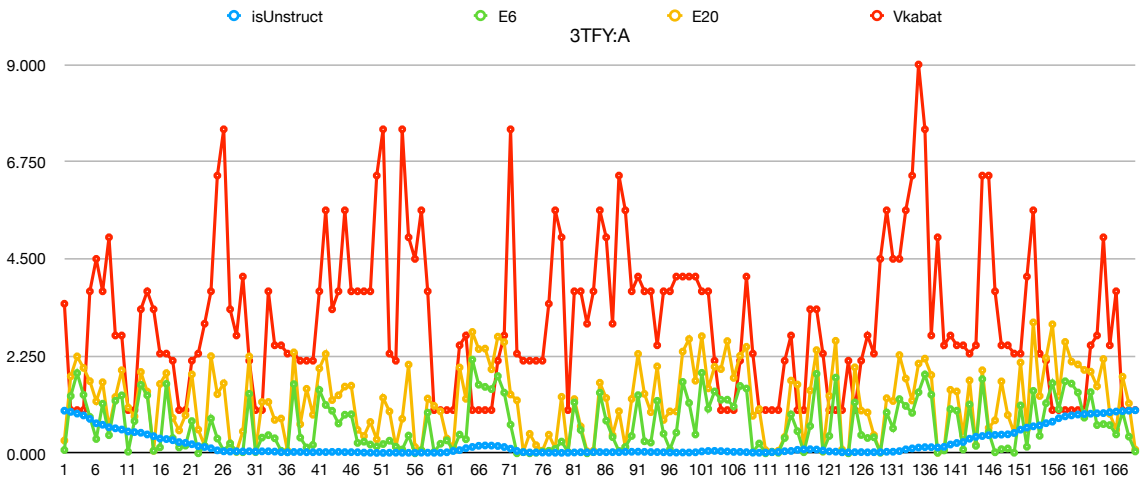


Figure E.35: Decriptors for 3W6S:A

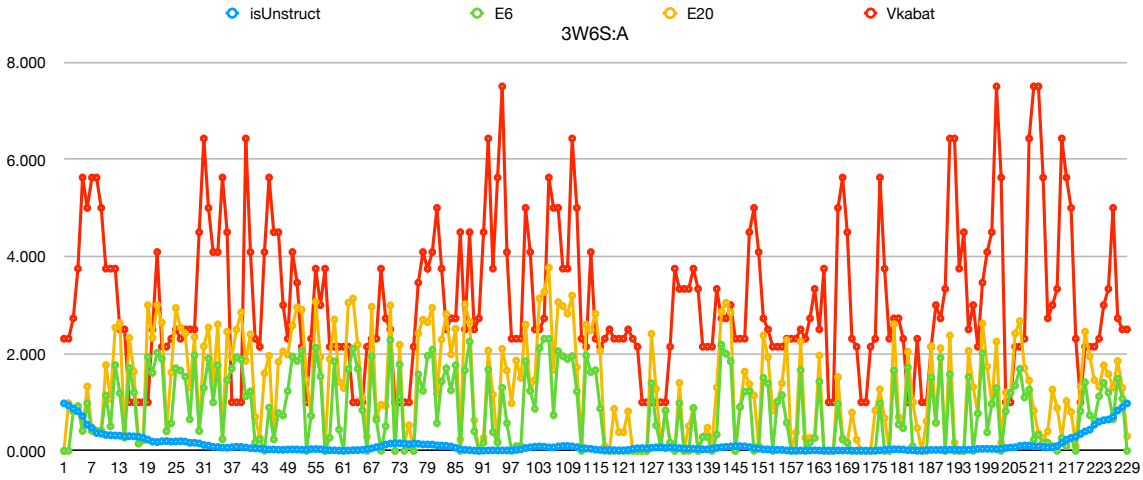


Figure E.36: Decriptors for 4AVA:A

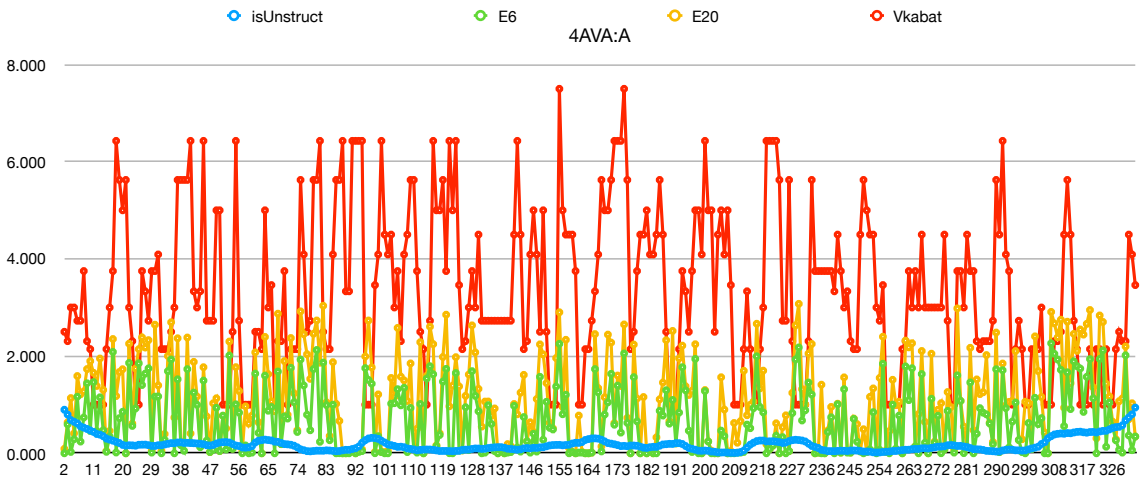


Figure E.37: Decriptors for 4EAB:A

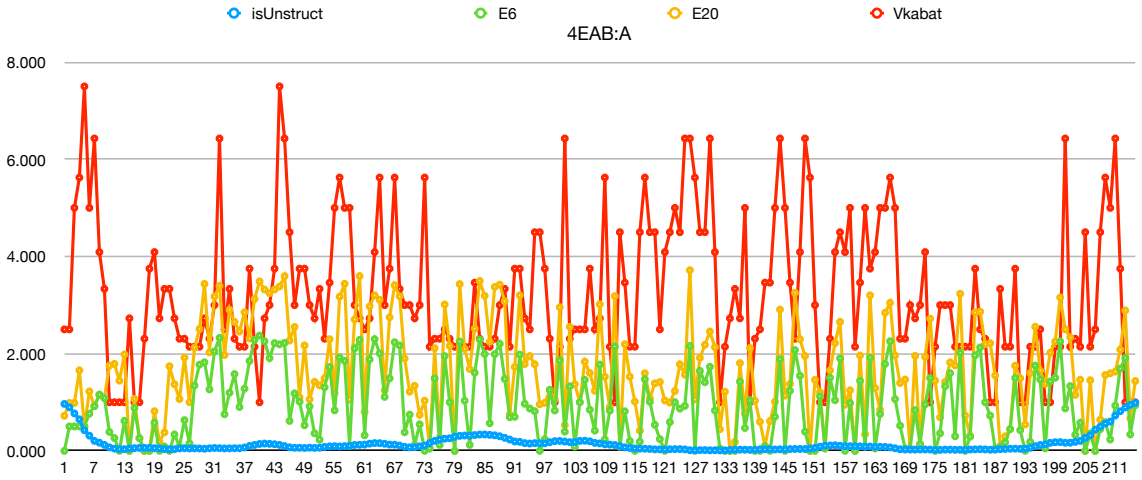


Figure E.38: Decriptors for 4FD4:A

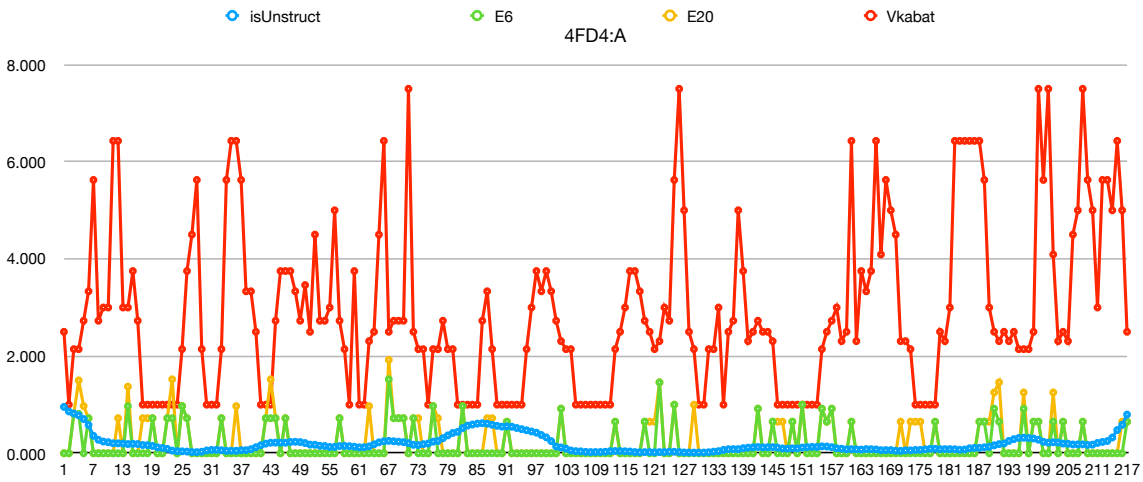


Figure E.39: Decriptors for 4FD5:A

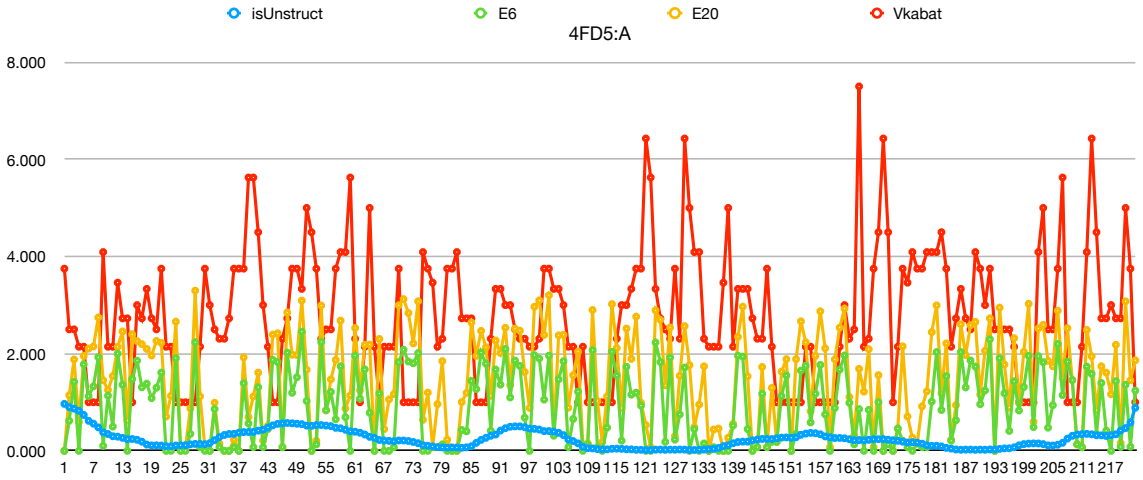


Figure E.40: Decriptors for 4FD7:A

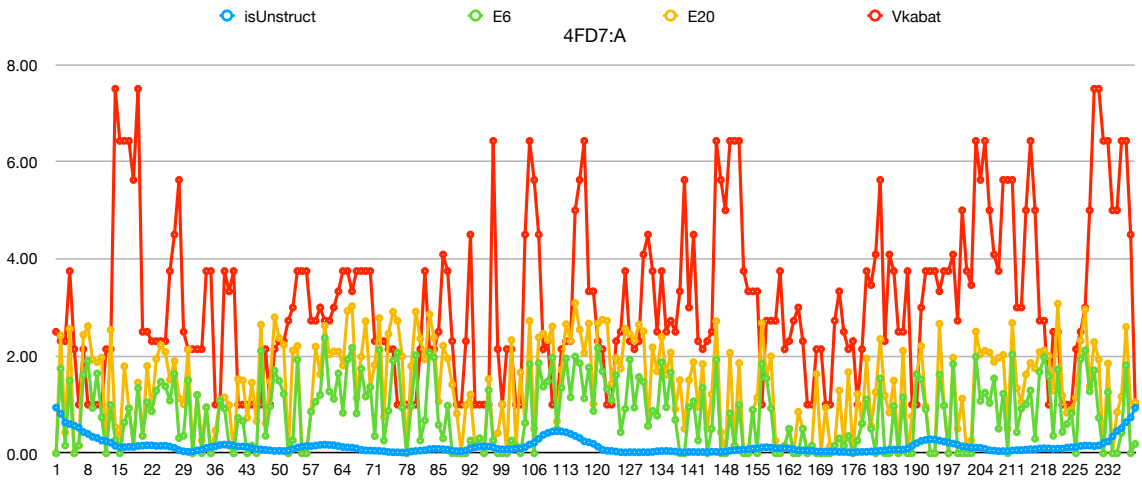


Figure E.41: Decriptors for 4HNY:A

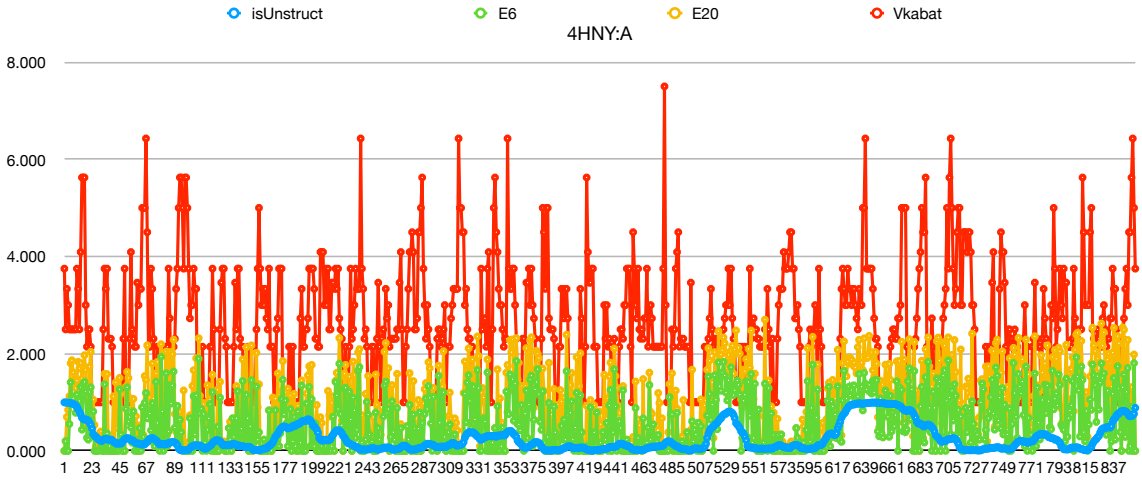


Figure E.42: Decriptors for 4J3G:A

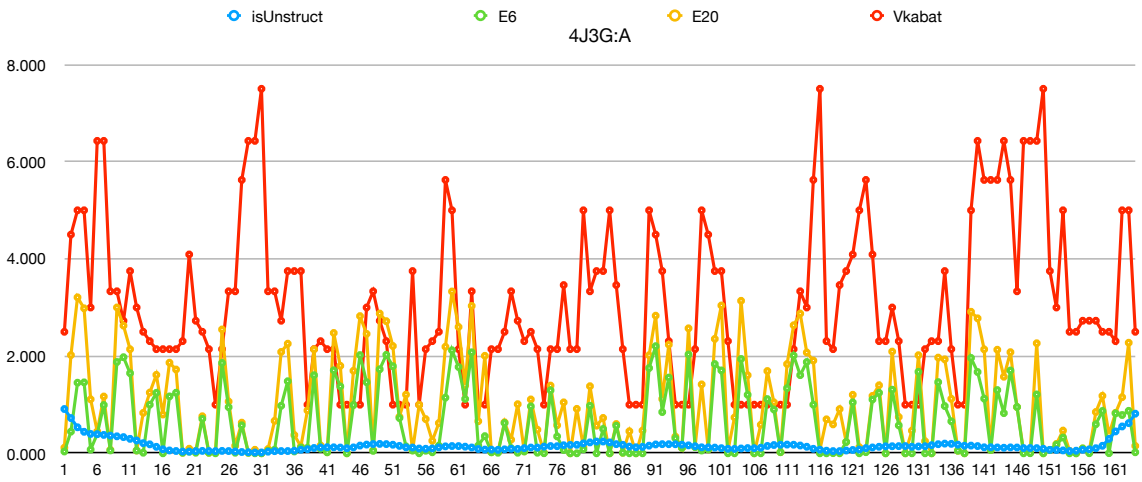


Figure E.43: Decriptors for 4JJX:A

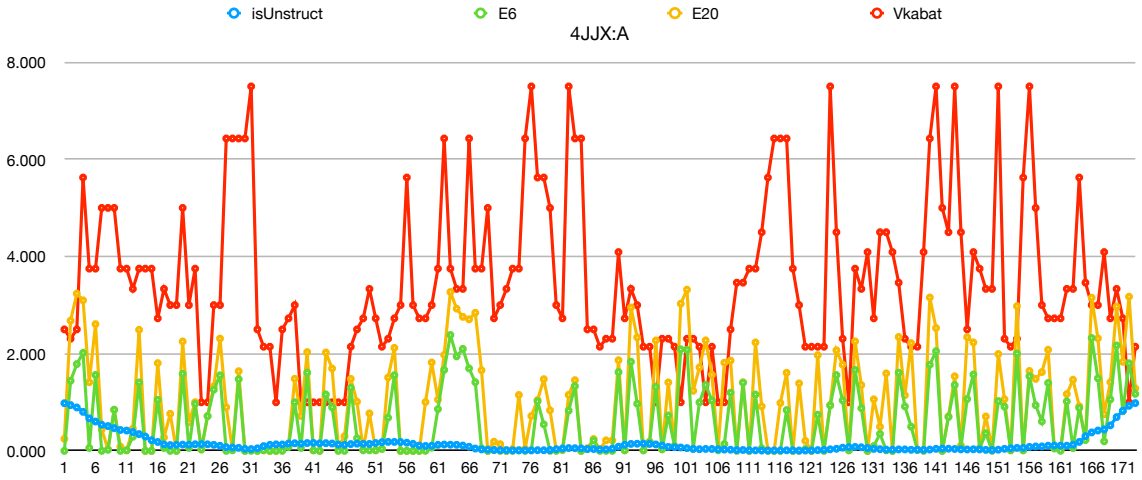


Figure E.44: Decriptors for 4KVO:A

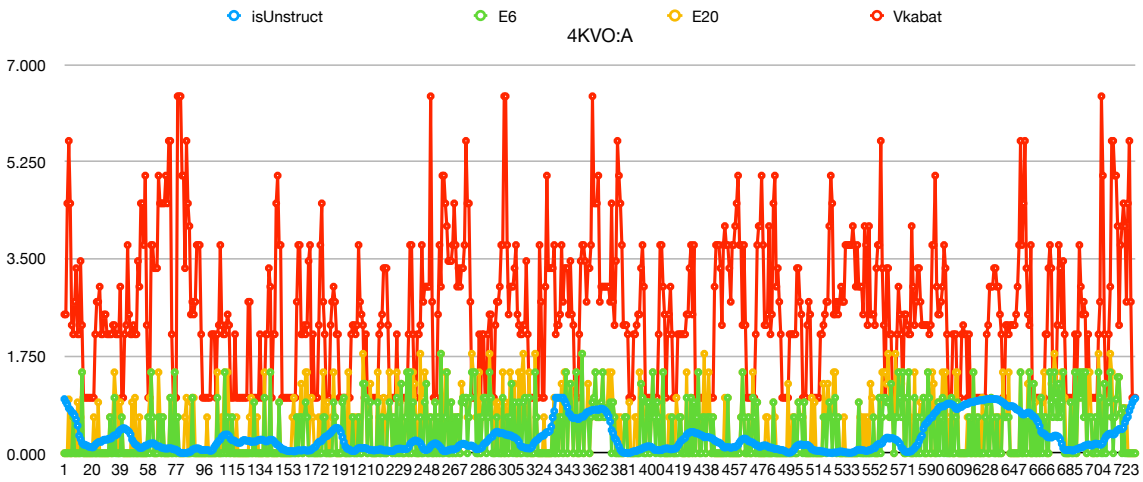


Figure E.45: Decriptors for 4KVX:A

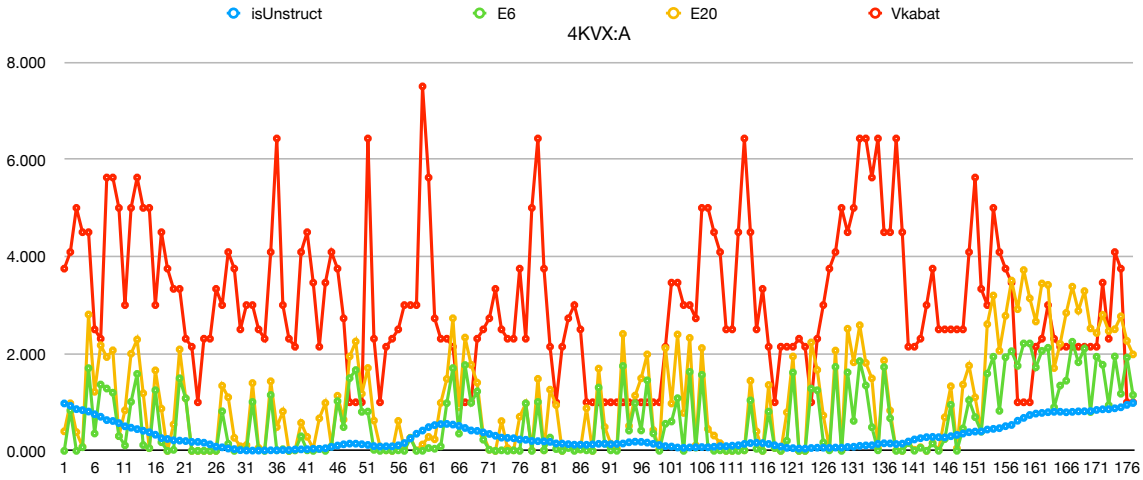


Figure E.46: Decriptors for 4PV6:A

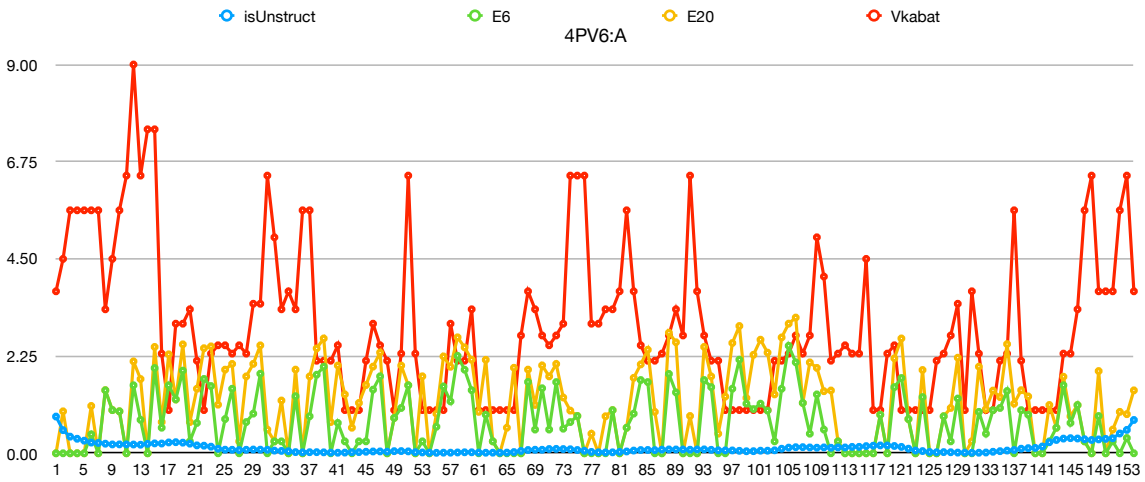


Figure E.47: Decriptors for 4R3K:A

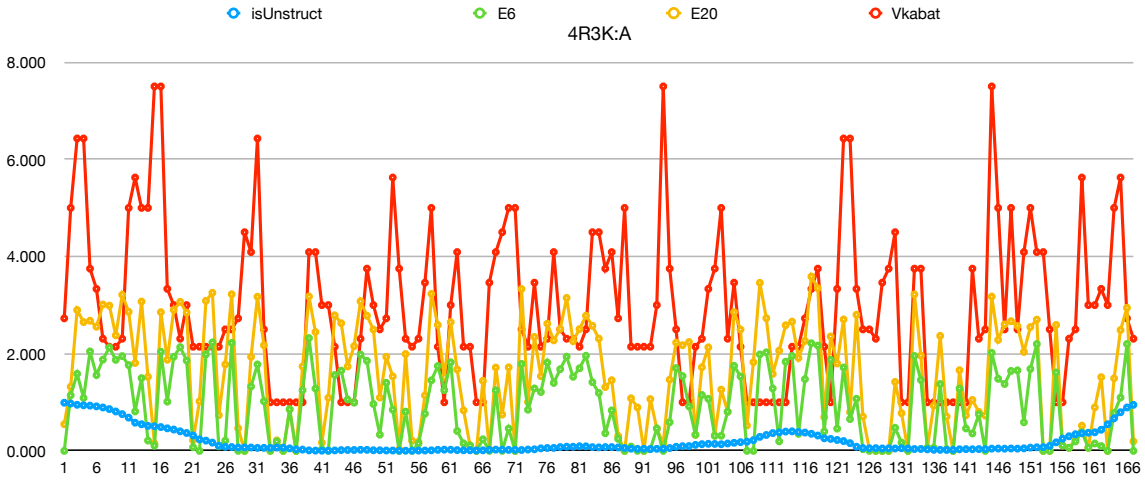


Figure E.48: Decriptors for 4R9M:A

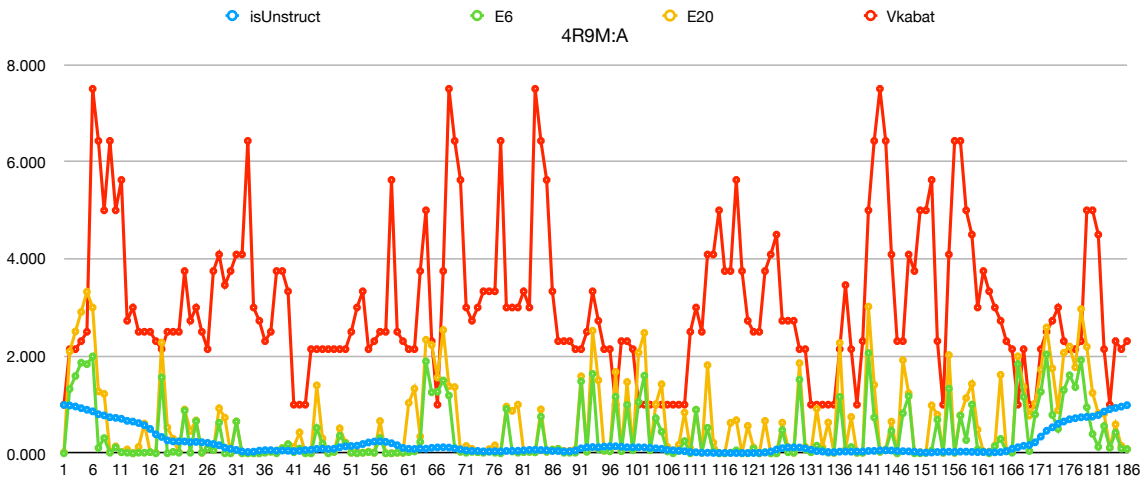


Figure E.49: Decriptors for 4RI1:A

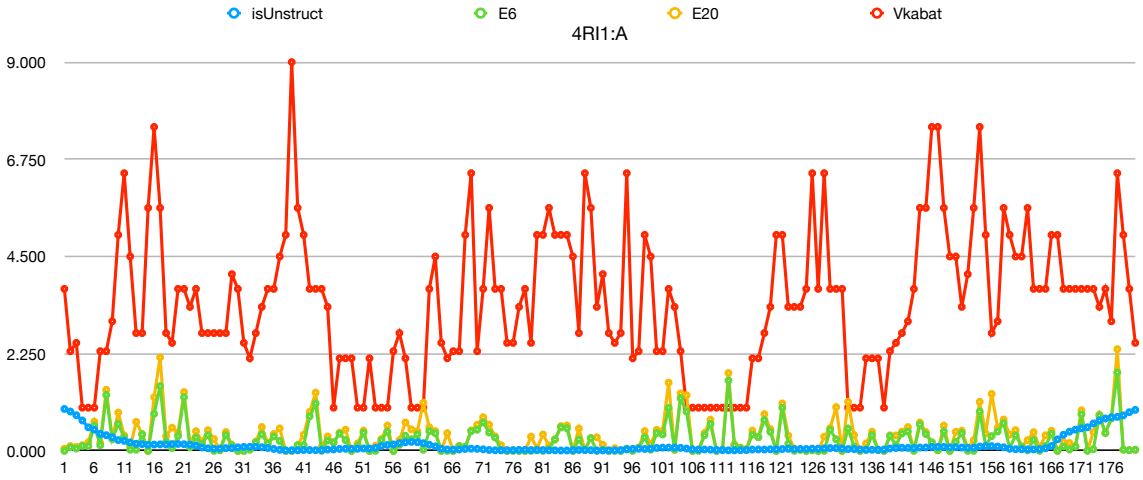


Figure E.50: Decriptors for 4U9V:B

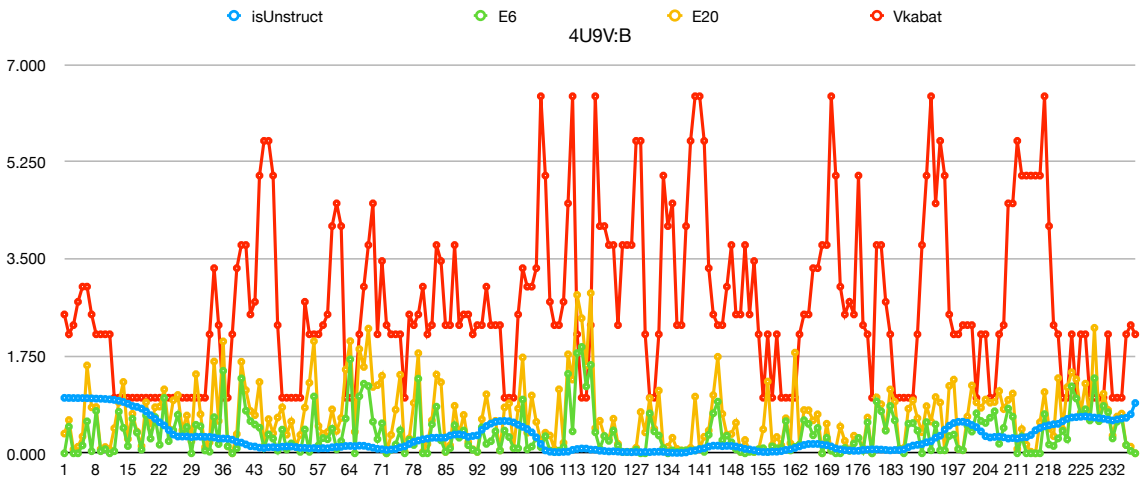


Figure E.51: Decriptors for 4UA3:A

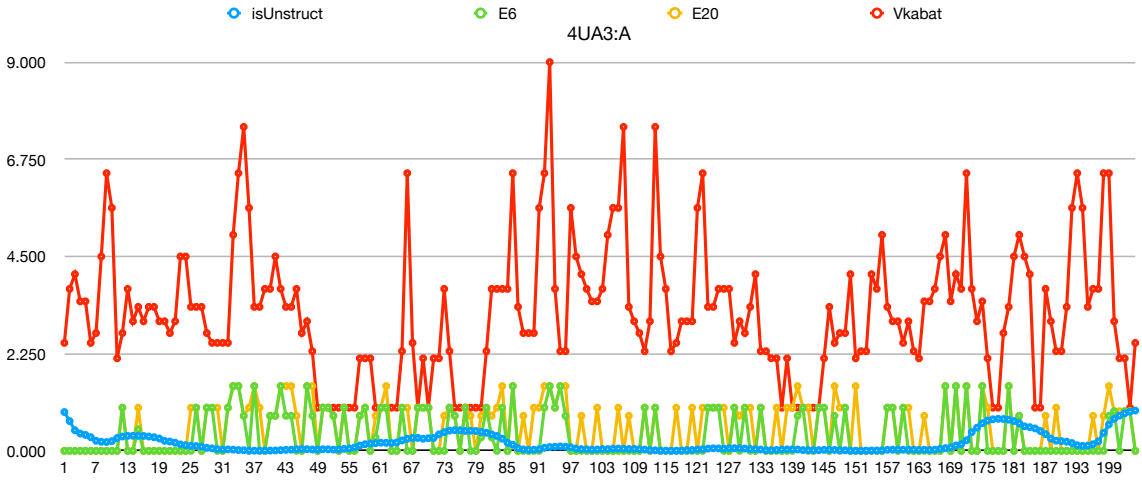


Figure E.52: Decriptors for 5GI5:A

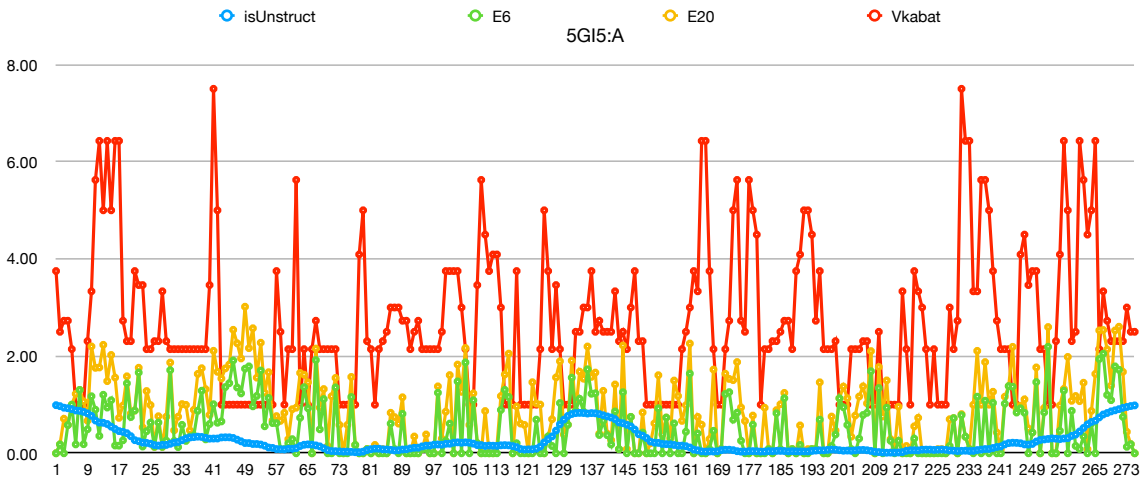


Figure E.53: Decriptors for 5HGZ:A

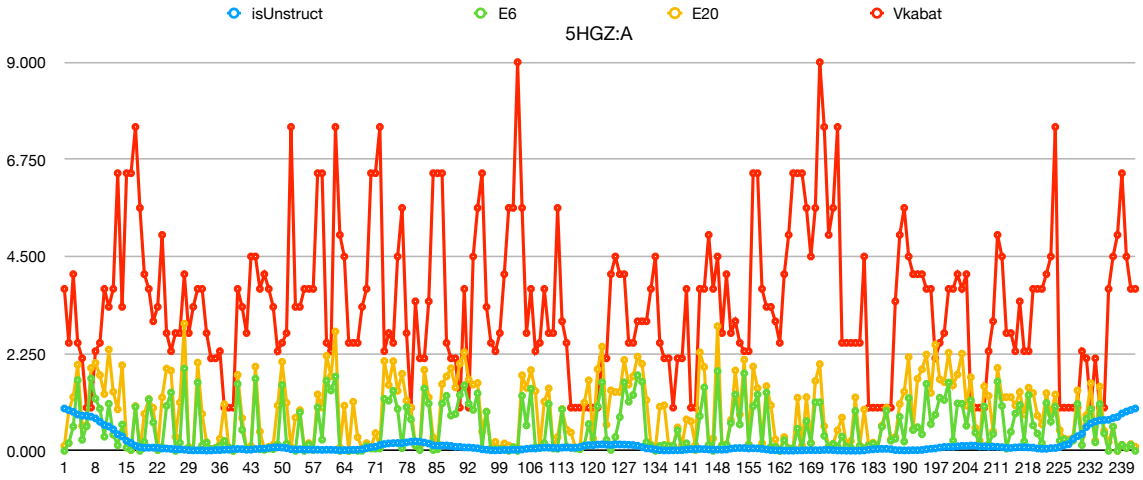


Figure E.54: Decriptors for 5JPH:A

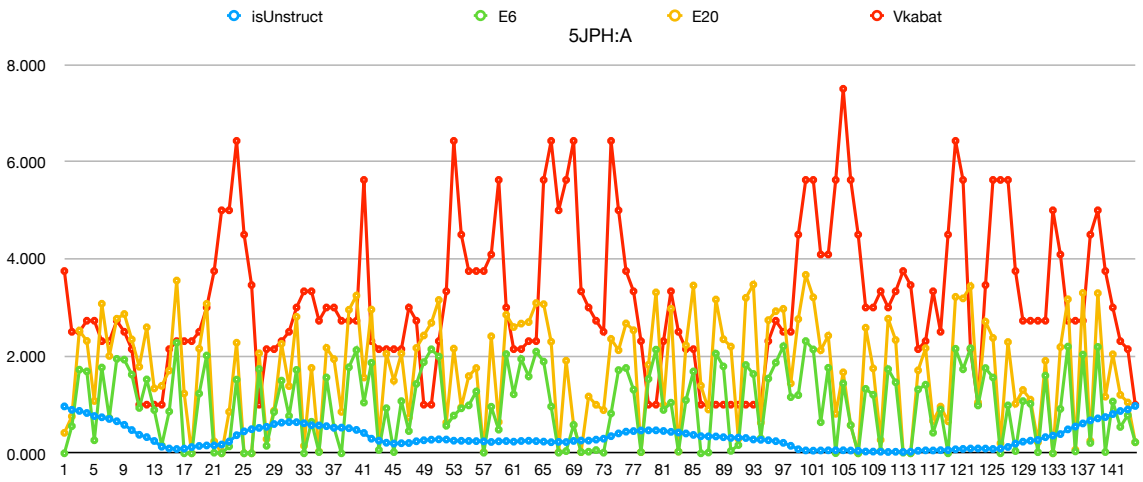


Figure E.55: Decriptors for 5K04:A

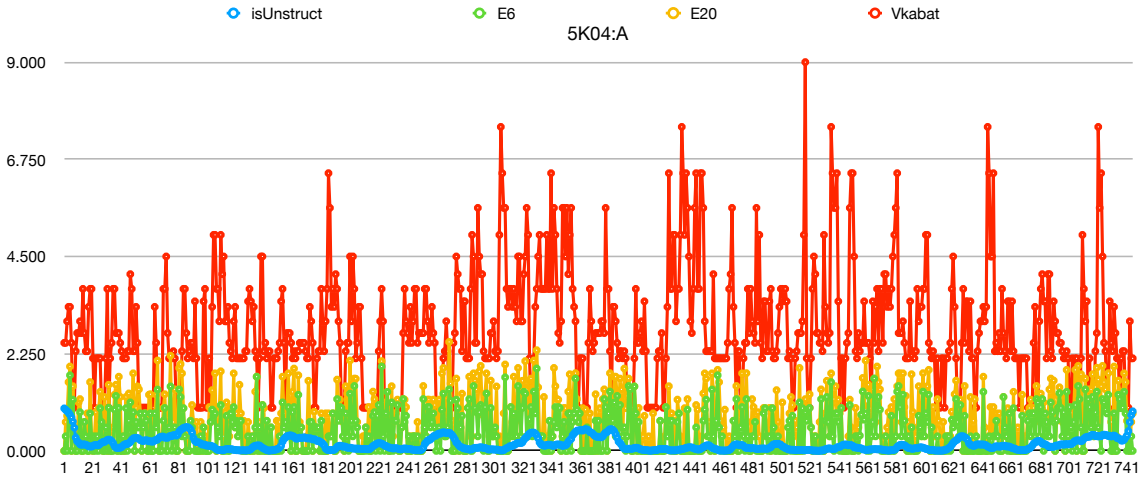


Figure E.56: Decriptors for 5K9N:A

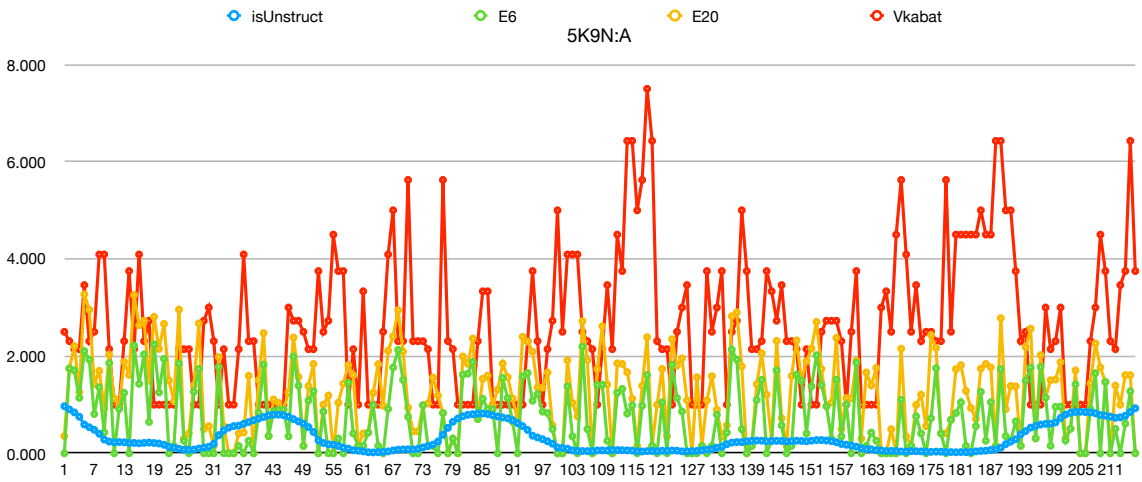


Figure E.57: Decriptors for 5KTA:A

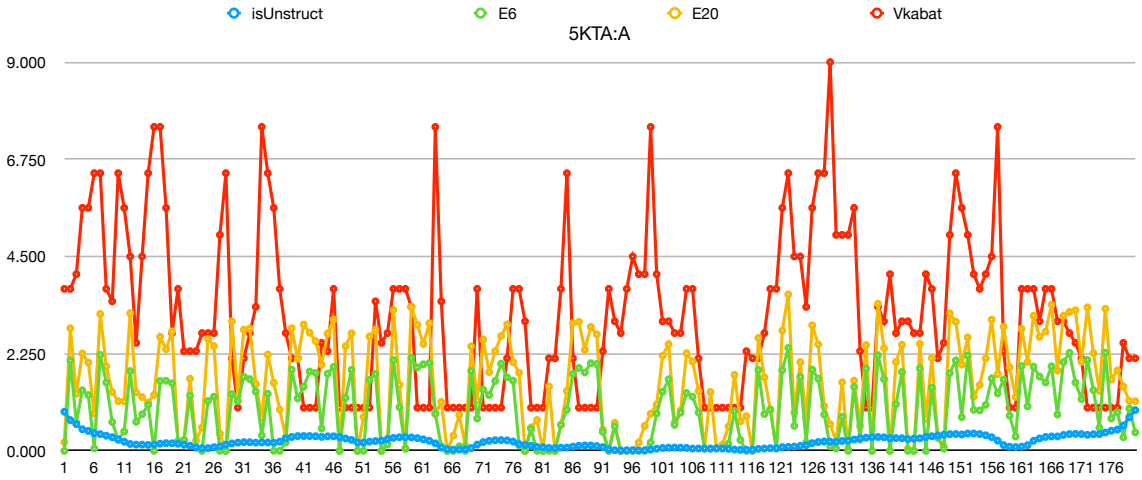


Figure E.58: Decriptors for 5WIF:A

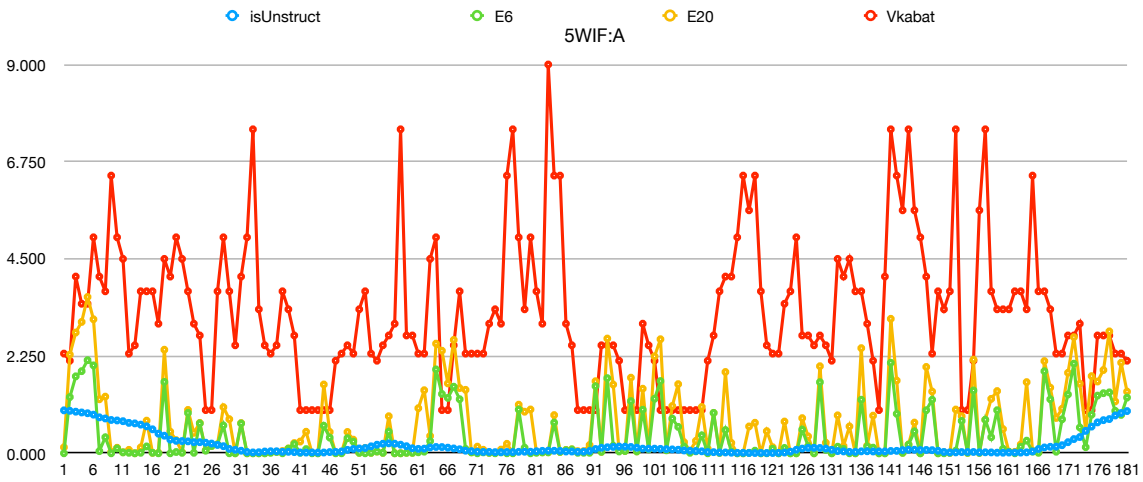
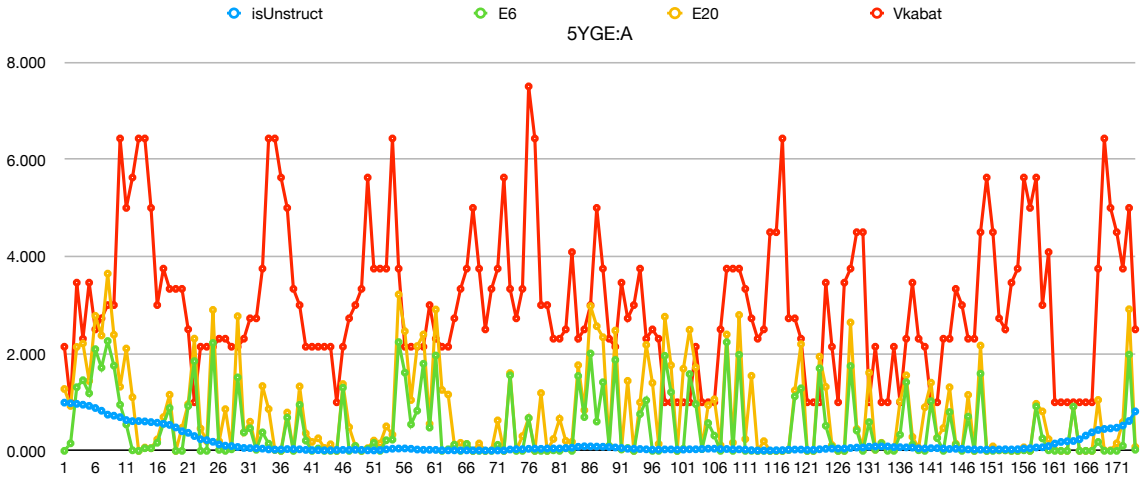


Figure E.59: Decriptors for 5YGE:A



E.2 Test Set

Figure E.60: Decriptors for 2B4Y:A

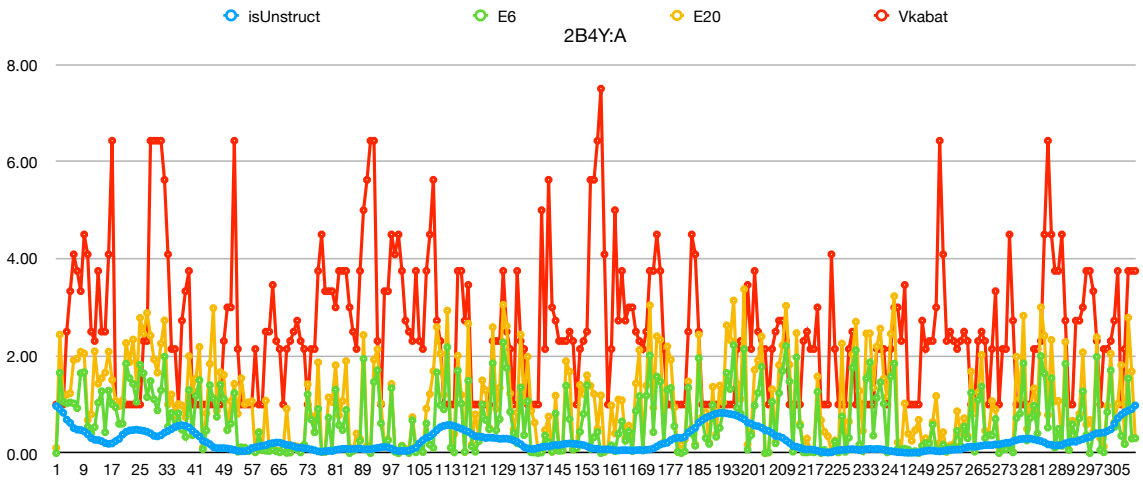


Figure E.61: Decriptors for 2HJH:A

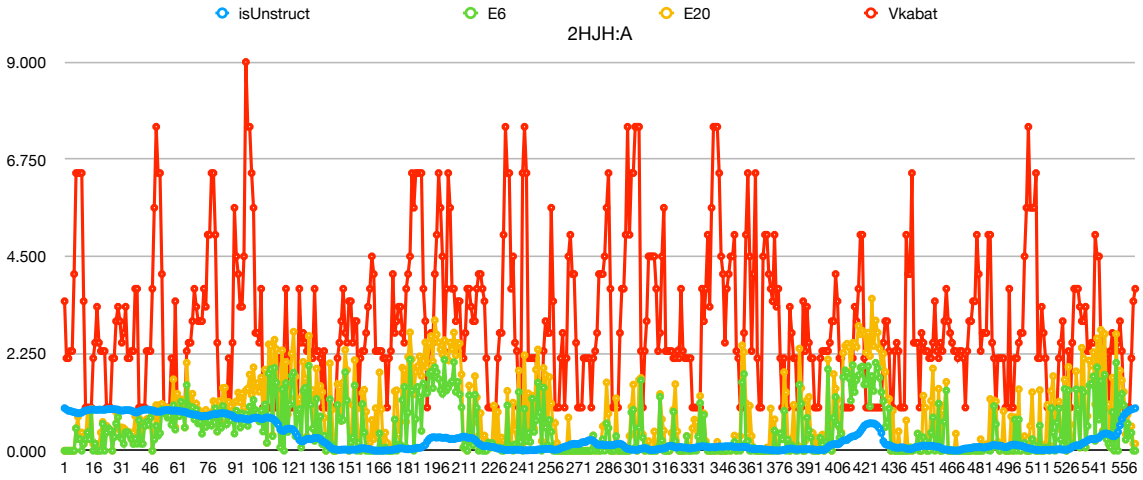


Figure E.62: Decriptors for 4IG9:A

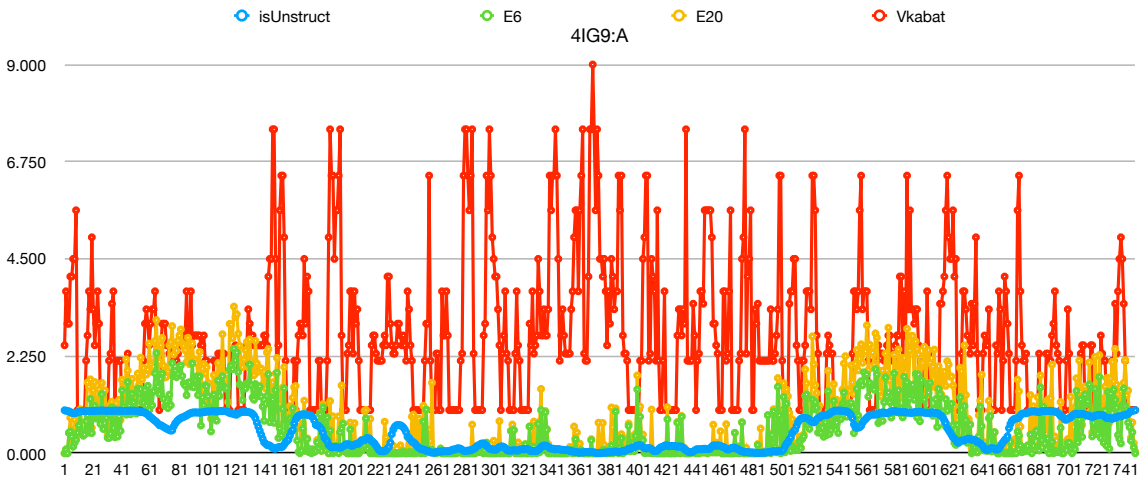


Figure E.63: Decriptors for 4L3O:A

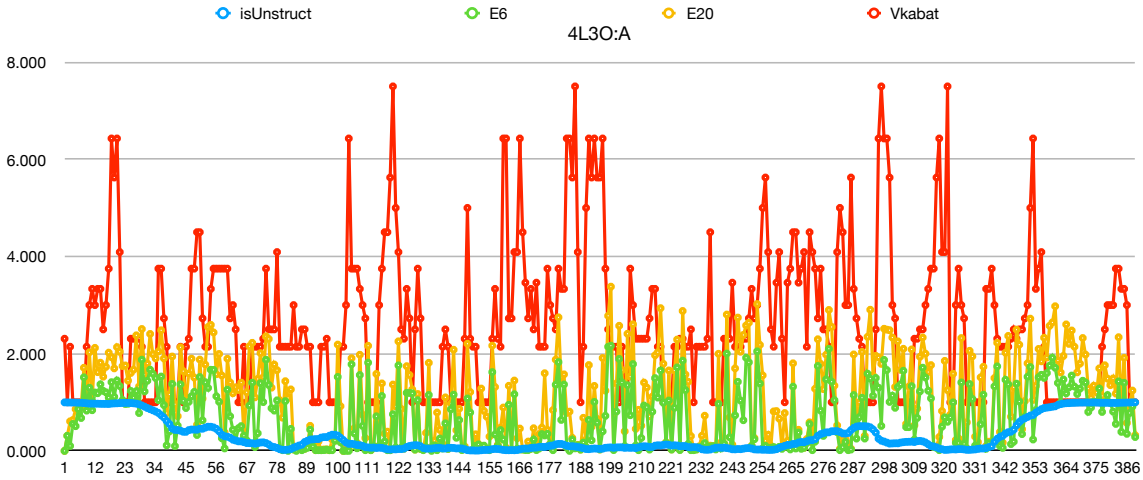
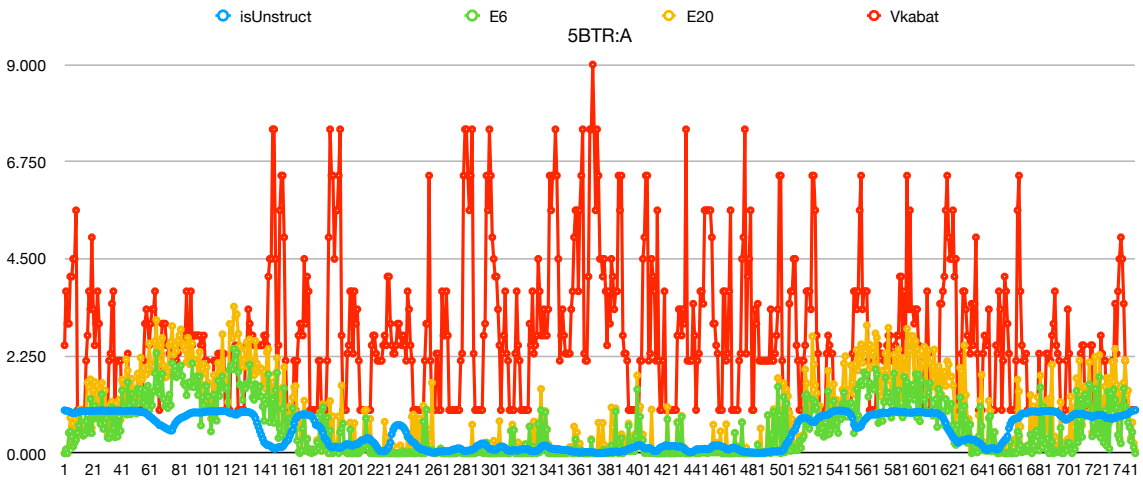


Figure E.64: Decriptors for 5BTR:A



APPENDIX F

Histograms

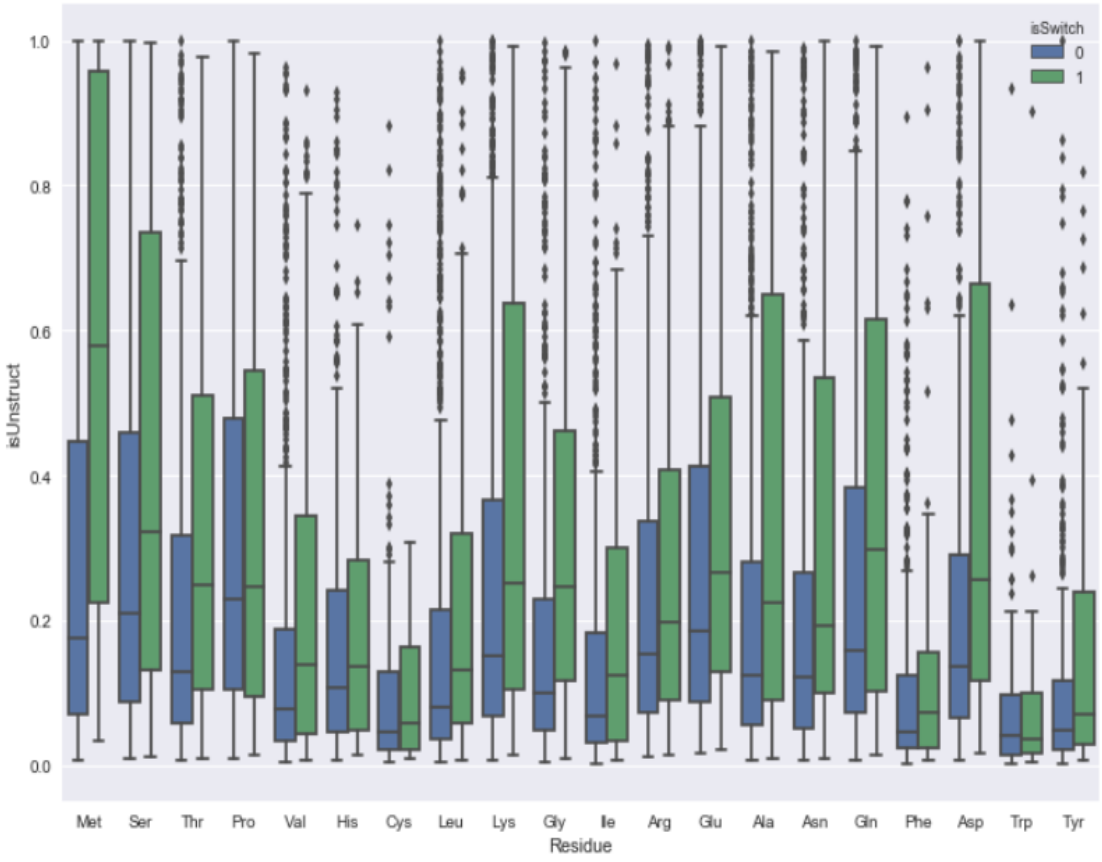


Figure F.65: IsUnstruct values from the learning set, broken down by residue type.

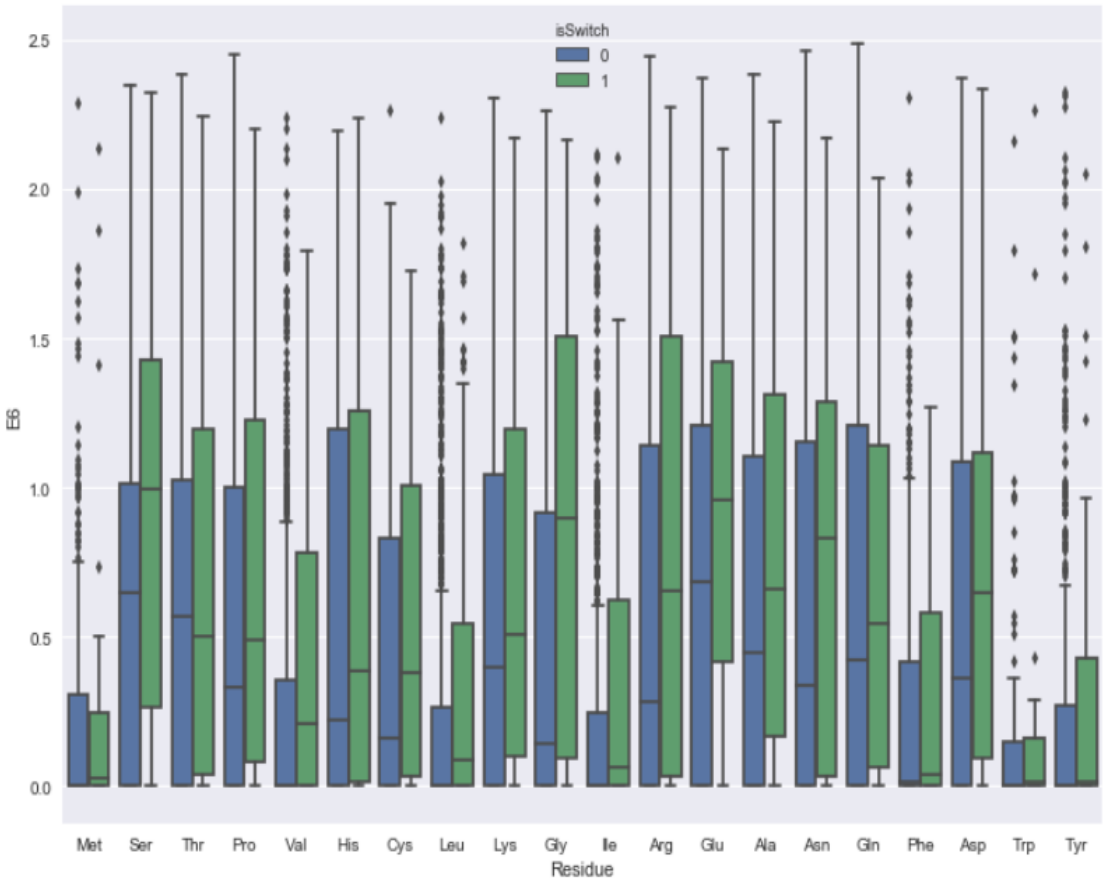


Figure F.66: E6 values from the learning set, broken down by residue type.

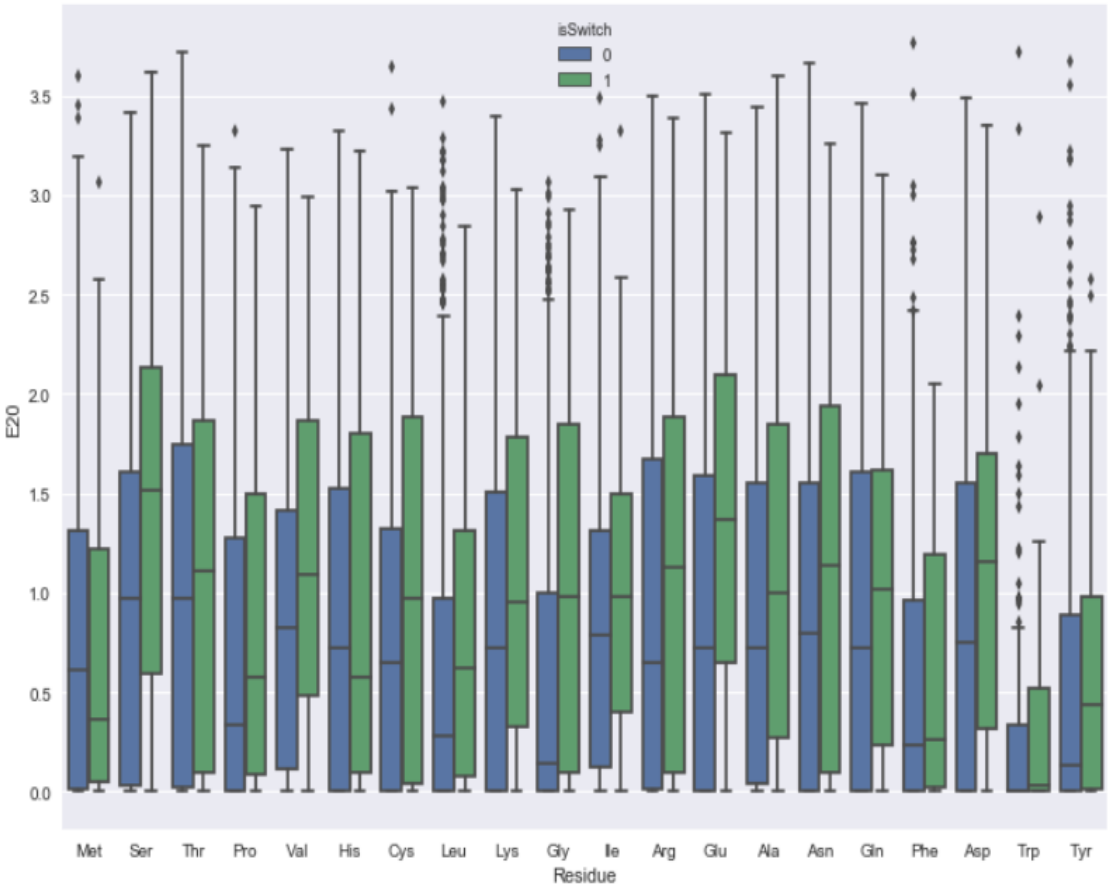


Figure F.67: E20 values from the learning set, broken down by residue type.

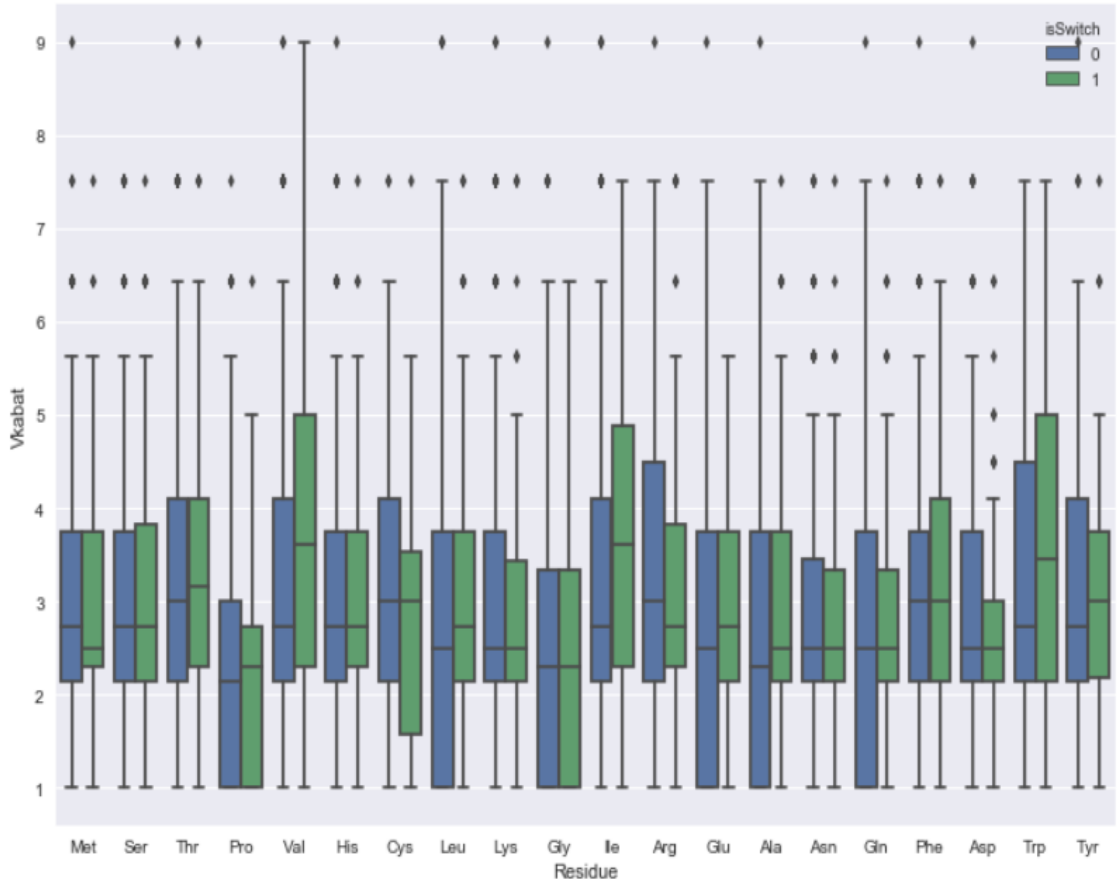


Figure F.68: IsUnstruct values from the learning set, broken down by residue type.